Particulate Matter Concentration Estimation from Satellite Aerosol and Meteorological Parameters: Data-Driven Approaches

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Abstract. Estimation of Particulate Matter concentration (PM_1 , $PM_{2.5}$ and PM_{10}) from aerosol product derived from satellite images and meteorological parameters brings a great advantage in air pollution monitoring since observation range is no longer limited around ground stations and estimation accuracy will be increased significantly. In this article, we investigate the application of Multiple Linear Regression (MLR) and Support Vector Regression (SVR) to make empirical data models for $PM_{1/2.5/10}$ estimation from satellite- and ground-based data. Experiments, which are carried out on data recorded in two year over Hanoi - Vietnam, not only indicate a case study of regional modeling but also present comparison of performance between a widely used technique (MLR) and an advanced method (SVR).

1 Introduction

Aerosol Optical Thickness/Aerosol Optical Depth (AOT/AOD) is considered as one of the Essential Climate Variables (ECV) [1] that influences climate, visibility and quality of the air. AOT is representative for the amount of particulates present in a vertical column of the Earth's atmosphere. Aerosol concentration can be measured directly by ground-based sensors or estimated from data recorded by sensors onboard polar and geostationary satellites observing the Earth. Ground measurements have usually high accuracy and temporal frequency (hourly) but they are representative of a limited spatial range around ground sites [2]. Conversely, satellite

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observation provides information at global scale with moderate quality and lower measurement frequency (daily).

MODerate resolution Imaging Spectrometer (MODIS) is a multispectral sensor on-board the two polar orbiting satellites Terra and Aqua, launched in 1999 and 2002, respectively and operated by the National Aeronautic and Space Administration (NASA). Using MODIS-measured spectral radiances, physical algorithms based on Look-Up Table (LUT) approaches have used since 90s to generate the aerosol products for Land and Ocean areas in Collection 004 [2] and following improved releases (Collection 005 [4], Collection 051 and the newest Collection 006 issued in 2006, 2008 and 2012, respectively). The aerosol product provided by NASA (MOD04L2) is trusted and largely used in many studies. However, its spatial resolution (10 km x 10 km) is appropriate for applications at the global scale but adequate for monitoring at regional scale. Therefore, an augmented AOT product, with spatial resolution of 1 km x 1 km, is obtained by PM MAPPER software package [3], of which quality has been validated over Europe using three year data [4].

The usage of satellite technology for air pollution monitoring applications has been recently increasing especially to provide global distribution of aerosol and its properties for deriving Particulate Matter concentration (PM), one of the major pollutants that affect air quality. PM is a complex mixture of solid and liquid particles that vary in size and composition and remain suspended in the air. PM is classified into PM₁, PM_{2.5} or PM₁₀ by their aerodynamic diameters. PM_{1/2.5/10} obtained by ground-based instruments has high quality and frequency but limited range, which makes the use of PM_{1/2.5/10} for monitoring air pollution at the global or regional scale become challenging. Motivated from early studies of relations between PM_{1/2.5/10} and AOT and the fact that satellite AOT nowadays has acceptable quality in comparison with ground-based AOT, thanks to technology achievements, deriving PM from satellite AOT is recently a promising approach.

In literature, relation between AOT and PM was considered over different areas (Italy, French, Netherland, United State, Peninsular Malaysia, Hong Kong, Sydney, Switzerland, Delhi, New York) in different experimental conditions [8, 10, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. The general methodology is applied using three main steps: (i) collecting satellite/ground-based AOT and ground-based PM_{2.5/10}; (ii) matching data following time and spatial constrains; (iii) investigating their relationship in different conditions. Experimental results showed that the relations are site-dependant, therefore they are not easy to be extrapolated to other locations. Besides, there are many factors effecting to PM estimation such as data collections, atmospheric conditions during studies, aerosol types and size fractionation, PM sampling techniques in which meteorological parameters are especially important. Ambient relative humidity, fractional cloud cover, mixing layer height, wind conditions, height of planetary boundary layer, temperature, pressure and wind velocity [12, 13, 14, 15, 16, 17, 18, 19] were considered seriously and used together with AOT in order to improve PM estimation accuracy.

Regarding estimation methodologies, Linear Regression (LR) or Multiple Linear Regression (MLR) are widely used to establish the AOD and $PM_{2.5/10}$ relationship, and therefore is regarded as a common and valid methodology to predict particulate

matters of different sizes (10 μ m and 2.5 μ m in diameter) [8, 10, 9, 10][15]. These techniques also applied to create mixed effect models in which meteorological parameters and land use information were used as input to PM prediction [18]. In a further improvement of the previous work, a robust calibration approach by integrating a simple adjustment technique into a mixed effect models is applied to estimate PM concentration using satellite AOD monthly average datasets [19].

Taking advantages of machine learning techniques, researchers have recently applied them to improve PM prediction. Exploited Self Organizing Map (SOM), Yahi et al. clustered integrated data by meteorological situations and then found high relationship between AOT and PM₁₀. Their experiments were applied to Lille region (France) for summer of the years 2003-2007 [20]. On a study using three years of MODIS AOT and meteorological data over southeast United State to estimate hourly or daily PM2.5, Artificial Neural Network (ANN) was able to improve regression coefficient R from 0.68 to 0.74 or 0.78, respectively in comparison with MLR [16]. Following the same approach, SVR is applied to estimate PM_{10} from satellite data, meteorological parameters and ancillary data over Austria in site domain (i.e. pixels around location of Austrian Air Quality ground-stations) and in model domain (i.e. the geographical domain of the Austrian Air Quality model). SVR implemented on a monthly basis in the period from 2008 to 2010 shows promising result in site domain (coefficient regression is bigger than 0.75) while further investigations should be done in model domain [21]. Originated from other sciences (Environment, Physics, Chemistry), the problem of PM estimation, which is started around 2002, has not considered the use of machine learning techniques seriously. The number of studies following the approach is limited although most of work done have shown promising results [16][20, 21].

In this article, we investigate the application of multiple linear regression and support vector regression to make empirical data models for $PM_{1/2.5/10}$ estimation from satellite aerosol product and ground-based meteorological parameters. Experiments over Hanoi, Vietnam, not only indicate a case study of regional modeling for PM_1 , $PM_{2.5}$, PM_{10} but also present performance of MLR, a widely used technique, and SVR, an advanced but investigated method.

The article is organized as follows. The methodologies including data collection, data integration and modeling techniques will be presented in Section 2. Experiments and results on data modeling of MLR and SVR will be described and discussed in Section 3. Finally, conclusions are given in Section 4, together with future works.

2 Methodologies

2.1 Data Collection

2.1.1 Satellite-Based Aerosol

The aerosol product provided by NASA, namely MOD04 L2, is derived from MODIS images using aerosol retrieval algorithms over land and ocean areas. These

methods match satellite observations to simulated values in LUT to derive aerosol concentration and its properties. Both algorithms perform on cloud-free pixels whose covered regions (land/water) are determined by their geographical information [2].

In an effort to improve the spatial resolution of the MODIS aerosol products, a software package called PM MAPPER was developed to increase spatial resolution from $10x10 \text{ km}^2$ to $3x3 \text{ km}^2$ and then $1x1 \text{ km}^2$. The PM MAPPER aerosol product at 3 km resolution was validated by direct comparison with MODIS retrievals and showed higher ability to retrieve pixels over land and coastlines [3]. The validation of the 1 km was carried out over Europe for the years 2007-2009. Comparison with both ground sun-photometers of the AERONET network and the MODIS 10 km AOT products have shown a high correlation [4]. In the article, PM MAPPER aerosol product (1 km spatial resolution) over Hanoi in two years is used in modeling and validation processes of PM_{1/2.5/10} estimation.

2.1.2 Ground-Based Aerosol

AERONET is the global system of ground based Remote Sensing aerosol network established by NASA and PHOTONS (University of Lille 1, CNES, and CNRS-INSU) (NASA, 2011). At AERONET stations, Aerosol Optical Thickness is measured by CIMEL Electronique 318A spectral radiometers, sun and sky scanning sun photometers in various wavelengths: 0.340, 0.380, 0.440, 0.500, 0.675, 0.870, 1.020, and 1.640 μ m in intervals of 15 minutes in average. After data processing steps, cloud-screened and quality-assured data are stored and provided as Level 2.0. In our work, AERONET aerosol product at level 2.0 are collocated in space and synchronized in time with satellite-based aerosols in order to validate the PM MAPPER AOT products over Hanoi, Vietnam.

2.1.3 Particulate Matter Concentration and Meteorological Data

Particulate matter suspended in the air is the main factor affecting to air quality and leading premature deaths. These fine particles have either anthropogenic sources (plants, burning of fossil fuels, spray can ...) or natural sources (dust storms, volcanoes, fires ...). Particles can be classified by size, referred to as fractions: PM_{10} , $PM_{2.5}$, PM_1 represent particles with aerodynamic diameters smaller than 10 μ m, 2.5 μ m and 1 μ m, respectively. Traditionally, particulate matter is measured directly at ground stations on hourly or daily basis. The ground measurements are highly trustworthy but not representative for areas far from ground stations.

In order to obtain PM measurements for modeling in Hanoi, we have used ground data provide by a station managed by Center for Environmental Monitoring (CEM) in Vietnam Environment Administration at geospatial coordinates (21°02'56.3", 105°22'58.8"). Data include particulate matter concentration at different sizes (1, 2.5 and 10 μ m) averaged by 24 hours and meteorological data (wind speed, wind direction, temperature, relative humidity, pressure and sun radiation) averaged by an hour in a period from August 2010 to July 2012.

2.2 Data Integration

Since data sets are collected from different sources, they have different temporal and spatial resolutions which can only be solved by an integration process. Satellite data include aerosol products at 1 km provided by the PM MAPPER. Ground-based measurements are obtained from the AERONET and CEM.

Satellite aerosol maps at 1 km of spatial resolution are obtained daily while $PM_{1/2.5/10}$, meteorological data and AERONET aerosol are measured at the ground stations and averaged in twenty-four hours, an hour and fifteen minutes in average, respectively. Time and location constrains are applied for data integration following the methodology proposed in [22]. Satellite data are considered if their pixels are cloudy-free and have distances to ground station within radius R. Meanwhile, contemporaneous measurements of AERONET and CEM instruments are selected and averaged within a temporal window T minutes around the satellite overpasses as illustrated in Fig. 1. The optimal thresholds of R and T will be selected by experiments presented in next sections.





2.3 Modeling Techniques

The modeling process is stated as follows. Given a training dataset including *l* samples:

$$\{(x_1, y_1), (x_2, y_2), \dots, (x_l, y_l)\} \in X \times Y$$
(1)

where *X*, *Y* denotes the space of the input and output patterns (i.e. $X \subset \mathbb{R}^n, Y \subset \mathbb{R}$). The modeling process would investigate an appropriate function *f* presented relationship between X_i and Y_i with the minimal error ε . The general form for the model would be as follows:

$$Y = f(X) + \varepsilon \tag{2}$$

In particular, the modeling process for PM estimation is to find an appropriate function f by applying a modeling technique on integrated datasets consisting of PM_{1/2.5/10}, AOT, Wind Speed (Wsp), Temperature (Temp), Relative Humidity (Rel_-H), Pressure (Bar) and sun Radiation (Rad). Multiple linear regression and support vector regression are considered in our work.

Multiple linear regression technique will assume f have a linear form and the problem become to estimate weighting parameters instead of the complicated infinite dimensional f. Based on MLR techniques, particulate matter concentration in different diameters is able to be calculated using equations as follows:

$$PM_{10} = \beta_0 + \beta_1 AOT + \beta_2 W sp + \beta_3 Temp + \beta_4 Rel H + \beta_5 Bar + \beta_6 Rad$$
(3)

$$PM_{2.5} = \alpha_0 + \alpha_1 AOT + \alpha_2 W sp + \alpha_3 Temp + \alpha_4 Rel H + \alpha_5 Bar + \alpha_6 Rad$$
(4)

$$PM_1 = \gamma_0 + \gamma_1 AOT + \gamma_2 W sp + \gamma_3 Temp + \gamma_4 Rel H + \gamma_5 Bar + \gamma_6 Rad$$
(5)

where PM₁₀, PM_{2.5}, PM₁ are PM mass concentrations (μ gm⁻³) and AOT is PM MAPPER AOT at 0.553 μ m (unit less). β_0 , α_0 , γ_0 are intercepts for PM₁₀, PM_{2.5}, PM₁ equations whereas β_{1-6} , α_{1-6} , γ_{1-6} are regression coefficients for the predictor variables including AOT, wind speed (ms⁻¹), temperature (C), relative humidity (%), barometer (hPa) and radiation (Wm⁻²).

The ε -SVR, firstly introduced by [23], will find a function f that has at most ε deviation from the actually obtained target Y from the training data in order to as 'flat' as possible to minimize the expected risk. In the case of linear SVR, flatness is to find the function f that presents an optimal regression hyper-plane with minimum slope w. In case of non-linear SVR, kernel functions are applied to map input space X into a high dimensional feature space F before construction of optimal separating hyper-planes in the high-dimensional space. The SVR problem is solved by the classical Lagrangian optimization techniques. Regarding PM estimation, the ε -SVR with epsilon loss function and Radial Basic Function (RBF) kernel provided by LIBSVM [24] is applied.

3 Experiments and Results

3.1 Satellite-Based Aerosol Validation

PM MAPPER provides AOT product at 1 km of spatial resolution using the improved MODIS aerosol algorithms. A validation over Europe was done on three years data and presented a high correlation in comparison to both ground sunphotometers of the AERONET network and the MOD04L2 AOT products [4]. Although PM MAPPER provides AOT maps at the global scale, this experiment is still carried out in order to validate its aerosol product at 1km over Hanoi before the modeling step.

In fact, as the CEM station hasn't provided any aerosol measurement, we used AOT collected from NghiaDo, the unique AERONET station in Hanoi. The NghiaDo station is far from the CEM station about 10 km in west, which is close enough to make an assumption that obtained aerosol is able to representative for both locations.

The PM MAPPER AOT maps and AERONET AOT measurements are collected in a year, from December 2010 to November 2011. A satellite map obtained daily is presented by three layer matrixes including latitude, longitude and AOT at 0.553 μ m. Each pixel is corresponding to 1km² area on the ground. Meanwhile, AERONET measurements provide AOT at various wavelengths: 0.340, 0.380, 0.440, 0.500, 0.675, 0.870, 1.020, and 1.640 μ m, in intervals of 15 minutes in average. All data are integrated following the method mentioned in Section 2.2 with various spatial window R and temporal window T. Different thresholds of R (10, 15, 20, 25, 30, 35, 40 and 50 km) and T (30, 60, 120 and 1440 minutes (~24 hours)) are considered in order to investigate satellite/ground-based aerosols behaviours. The



Fig. 2 (a) Correlation Coefficient and (b) Root Mean Square Error between PM MAPPER AOT and AERONET AOT

validation results are presented in Fig. 2. CORrelation coefficient (COR) increases by spatial and temporal windows (Fig. 2(a)) while Root Mean Square Error (RMSE) decreases by distance but has the same behaviours if temporal windows at 60, 120 minutes or all day are applied (Fig.2(b)). The best match should be established between satellite AOT collected in areas of 25 km around the AERONET station and ground-based AOT averaged in a day when the satellite image is recorded. In this case, we obtained PM MAPPER AOT and AERONET AOT's COR = 0.648 and RMSE = 0.421, which is good enough for using PM MAPPER AOT in $PM_{1/2.5/10}$ estimation.

3.2 Threshold Selection

In this section, we present an experiment to identify spatial and temporal thresholds for integration data in order to obtain samples for the $PM_{1/2.5/10}$ modeling step. Data

collected from August 2010 to July 2012 consist of daily AOT maps at 1 km^2 , daily particulate matter concentration (PM₁, PM_{2.5}, PM₁₀) and hourly meteorological parameters (wind speed, temperature, relative humidity, pressure and sun radiation). The experiment is carried out to integrate data with various spatial windows for AOT maps (R=5, 10, 15, 20, 25, 30, 35, 40, 45 and 50km) and different temporal windows for meteorological data (the nearest time - T1, average of two nearest times - T2 and average of four nearest times - T3). Correlation coefficient matrixes for all parameter are calculated to investigate relations among them. However, no much difference can be found with various temporal windows, and therefore we selected the temporal threshold T1 and only present its results.

The Fig. 3 presents correlation coefficient between AOT collected at many distance thresholds and other variables on experimental datasets. AOT-PM₁₀, AOT-PM_{2.5} and AOT-PM₁ correlation are optimal at 35, 30, 30 km, respectively. However, the threshold of 30 km should be selected because it almost maximizes all considered correlations (COR of AOT-PM₁₀ = 0.301, COR of AOT-PM_{2.5} = 0.255 and COR of AOT-PM₁ = 0.192). Regarding meteorological parameters, AOT relationship is strong with relative humidity (Rel_H.), weak with wind speed, sun radiation (Wsp., Rad.) and almost not with pressure and temperature (Bar., Temp.) (see Fig. 3).



Fig. 3 Correlation Coefficients in distance between satellite AOT and other factors

From data sets selected by proposed spatial and temporal thresholds (R= 30km, T=T1), we carried out a further experiment to investigate which factors will be important to PM₁₀, PM_{2.5}, PM₁ estimation in the modeling step. CORs are calculated between PM_{1/2.5/10} and other variables. Results presented in Fig. 4 show that dependence of PM on AOT increases in the order of their aerodynamic diameters (i.e. 1, 2.5 and then 10 μ m) whereas their relations of PM with meteorological variables (Wsp., Temp., Rel_H., Bar. and Rad.) decreases with their size (i.e. 10, 2.5 and then 1 μ m). The obtained results confirmed that satellite AOT is a key factor. Besides, temperature, radiation and wind speed should affect to data models more strongly than relative humidity and pressure. However, considering together with CORs between AOT and other factors (Fig. 3), we decided to use all meteorological parameters in the next modeling step.



Fig. 4 Correlation coefficients between PM_{1/2.5/10} and other factors in the selected dataset

3.3 MLP and SVR Comparison

MLP and SVR techniques presented in Section 2.3 are applied to estimate $PM_{1/2.5/10}$ values. The experiment focuses on investigating estimators of different types of particle mass concentration (PM_1 , $PM_{2.5}$ and PM_{10}), role of satellite AOT and performance of two regression methodologies. Data for each type of PM are obtained by using thresholds proposed in the previous section. They are grouped into two years (August 2010 - July 2011 and August 2011 - July 2012) with statistics shown in Fig. 5. In two years, the totals of samples are comparable (55,131 and 49,908) but data distributions over many months are too much different (Aug, Oct, Nov, Jan, Feb, Mar and Apr). Therefore, we considered data in year basis instead of month or season basis as mentioned in previous studies. Moreover, datasets with (w) and without (w/o) satellite AOT are created and considered in our experiment. One year data is used for training whereas another year data is used to testing and vice versa. The final COR and RMSE are averaged on two year results for each PM₁, PM_{2.5} and PM₁₀ (see Table 1).



Fig. 5 Statistics on total data sets

	PM10			PM _{2.5}			PM ₁		
	MRL- w/o	MRL-w	SVR-w	MRL- w/o	MRL-w	SVR-w	MRL- w/o	MRL-w	SVR-w
COR	0.038	0.174	0.239	0.429	0.598	0.593	0.608	0.659	0.694
RMSE	109.225	96.656	74.935	40.836	31.071	31.674	24.591	22.939	22.349

Table 1 MLR and SVR performance on PM₁₀, PM_{2.5} and PM₁ estimation

Regarding types of particle mass concentration, PM_1 can be estimated best by both MLR and SVR techniques (COR/RMSE = 0.659/22.939 and 0.694/22.349, respectively). $PM_{2.5}$ estimation is following with MLR COR/RMSE at 0.598/31.071 and SVR COR/RMSE at 0.593/31.674. The worst case is for PM_{10} estimation (MLR COR/RMSE = 0.174/96.656 and SVR COR/RMSE = 0.239/74.935). Based on experimental results, PM_1 and $PM_{2.5}$ estimation seem good enough while PM_{10} estimation need more data for modeling and further investigation.

The use of satellite AOT in $PM_{1/2.5/10}$ prediction is able to improve regression correlation and accuracy significantly. In case of PM_{10} estimation, regression correlation increases from 0.038 to 0.174 and 0.239 when MLR and SVR are applied. COR of $PM_{2.5}$ estimation increases from 0.429 to 0.598 and 0.593 while the same trend is also seen on PM_1 estimation (from 0.608 to 0.659 and 0.694, respectively). The strong improvement is happened to PM_{10} than $PM_{2.5}$ or PM_1 estimators. It can be explained by the different levels of relation between $PM_{1/2.5/10}$ and AOT as shown in Fig. 4.

In comparison of modeling techniques performance using datasets with satellite AOT, SVR is better than MRL for PM_{10} and PM_1 estimation. The regression correlation increases 36.9% and 5.5% while error decreases 22.4% and 2.6%, respectively. Meanwhile, MRL and SVR perform in nearly same way for $PM_{2.5}$ estimation, which is presented by a slight difference of COR (0.78%) and RMSE (1.9%). In general, SVR outperforms MLR in our experiments although its improvements are not impressive as shown in other studies [16][21]. It could be due to different datasets and data splitting methods. In the experiment, our data are limited on a CEM station and so, divided by years instead of locations. Therefore, the problem of $PM_{1/2.5/10}$ estimation becomes a more challenging task, $PM_{1/2.5/10}$ prediction.

4 Conclusion and Future Works

In this article, we presented estimation methodologies of PM_1 , $PM_{2.5}$ and PM_{10} from satellite AOT product and meteorological parameters (wind speed, temperature, relative humidity, pressure and radiation) using MLR and SVR techniques applied on integrated data in two years from August 2010 to July 2012 over Hanoi, Vietnam.

Experiments are carried out to investigate estimation of different types of particle mass concentration (PM_1 , $PM_{2.5}$ and PM_{10}), role of satellite AOT and performance of two regression methodologies. Results showed that estimation quality decreases by PM_{10} , $PM_{2.5}$ and PM_1 as results of loose relationship of PM_{10} on meteorology parameters in comparison with $PM_{2.5}$ and PM_1 . However, the use of satellite AOT in

modeling is able to improve all PM estimators accuracy. For regression techniques, SVR outperforms MLR but more data collection, ground station extension and further investigation should be done. The presented work can be considered as a case study for regional $PM_{1/2.5/10}$ models over Hanoi, Vietnam.

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