A Data-Mining Approach for the Validation of Aerosol Retrievals

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***Abstract*—Operational algorithms for retrieval of aerosols from satellite observations are typically created manually based on the domain knowledge. Validation studies, where the retrievals are compared to the available ground-truth data, are periodically performed with the goal of understanding how to further improve the quality of the retrieval algorithms. This letter describes a data-mining approach aimed to facilitate this highly labor-intensive process. It is based on training a neural network for retrieval and comparing its performance with that of the operational algorithm. The situations, where a neural network is more accurate, point to the weaknesses of the operational algorithm that could be corrected. Use of decision trees is proposed to provide easily interpretable descriptions of such situations. The approach was applied on 3646 collocated Moderate Resolution Imaging Spectroradiometer and AERONET observations over the continental U.S. related to the retrieval of aerosol optical thickness. The experiments showed that the approach is feasible and that it can be a valuable tool for the domain scientists working on the development of retrieval algorithms.**

***Index Terms*—Aerosol Robotic Network (AERONET), aerosols, data mining, decision trees, Moderate Resolution Imaging Spectroradiometer (MODIS), neural networks (NNs), retrievals.**

I. Introduction

AEROSOLS are small particles emanating from natural and man-made sources that both reflect and absorb incoming solar radiation. One of the biggest challenges of current climate research is to characterize and quantify the effect of aerosols on the Earth's radiation budget [1]. There are two major types of instruments that collect aerosol data, such as the following: 1) satellite instruments, such as AVHRR-2, GOME, TOMS, PONDER, MISR, and Moderate Resolution Imaging Spectroradiometer (MODIS) [2] and 2) ground-based instruments, represented by the Aerosol Robotic Network (AERONET) [3], a global network of about 180 operational sun/sky radiometers. Satellite instruments provide global coverage with high spatial resolution, relatively low temporal resolution, and moderately accurate retrievals. AERONET has limited spatial coverage, relatively large temporal resolution, and highly accurate retrievals. As a result, AERONET is often used to validate satellite-based retrievals.

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Since 2000, the MODIS instrument aboard the TERRA satellite has been a major source of high-quality aerosol information. The operational MODIS aerosol-retrieval algorithm is an inverse operator of a high-dimensional nonlinear function represented by a forward-simulation model, which is derived according to the domain knowledge about aerosol physical properties. The algorithm derives the aerosol optical thickness (AOT) by matching the observed spectral reflectance at the top of the atmosphere to the simulated values stored in lookup tables.

Validation of MODIS retrievals showed that they are more accurate over oceans than over land [4]. For retrievals over land, the errors were estimated to fall within a range of $\pm(0.2\text{AOT} + 0.05)$ over a global scale [5]. A more detailed look reveals large variability in the retrieval quality as a function of location, season, prevalent aerosol type, and aerosol loading. For example, the MODIS algorithm exhibited high bias during the dust-load periods over India [6] due to a reduction in the difference between the surface and atmospheric forcing. The underestimation of AOT at higher aerosol loadings in certain parts of Africa was attributed to insufficient light absorption in the aerosol models [7].

Overall, the main sources of MODIS aerosol-retrieval errors are the separation of surface and atmospheric components of the observed radiances, the inaccuracies in the forward-simulation model, and inversion errors. Some sources of retrieval uncertainties, such as bright surfaces or cloud-contaminated scenes, are due to the limitations of the MODIS instrument and cannot be corrected, while others, such as imperfections in the retrieval algorithm, are correctable. A goal of aerosol scientists is to understand the primary sources of correctable retrieval errors and to use such knowledge to improve the retrieval algorithms. The goal of this letter is to explore if data mining could facilitate this process.

Our approach has the following three main components: 1) use collocated AERONET and MODIS data to train neural networks (NNs) for the retrieval of AOT; 2) compare the accuracy of NNs and the MODIS operational algorithm; and 3) understand the conditions when the NN is more accurate than MODIS retrievals.

A neural network trained in the first step is a completely data-driven retrieval algorithm, distinct from the modeldriven MODIS operational algorithm. A property of NN retrieval is that its high accuracy is guaranteed only for the conditions similar to those at the AERONET sites. As such, neural networks should not be used for the operational retrievals. However, if NNs can achieve higher retrieval accuracy over the AERONET locations, it becomes evident that the MODIS algorithm can be further improved.

The proposed approach is evaluated using collocated aerosol data covering the continental U.S. between 2002 and 2004. This choice is justified because some of the poorest retrieval results were observed along the east coast of the U.S. at the blue wavelength, where less than 60% of the retrievals fell within expected error bars [8]. Furthermore, the western U.S., where AERONET stations are mostly located over coastal and desert regions, are also characterized by a larger than average MODIS retrieval error [9].

II. Data Sets

A. AERONET Data

The AERONET is a globally distributed network of automated ground-based instruments and data archives, developed to support aerosol scientists. The instruments used are CIMEL spectral radiometers that measure direct-sun and diffuse-sky radiances and determine AOT in seven spectral bands (340, 380, 440, 500, 670, 870, and 1020 nm). AERONET retrievals are very accurate and are widely used for the validation of satellite-based AOT retrievals.

We obtained level-1.5 cloud-screened AERONET AOTs for 36 sites (see Figs. 2 and 3) in the continental U.S. between January 2002 and December 2004. Since there are no AERONET AOT measurements at the MODIS wavelengths of 470 and 660 nm, these values have been interpolated from the values at 440 and 870 nm, assuming the log-linearity in the range [8].

B. MODIS Data

MODIS is a key instrument aboard the TERRA satellite for the collection of aerosol and cloud information. MODIS has a swath width of 2330 km and achieves global coverage in about two days. The MODIS instrument has a single camera observing top-of-the-atmosphere reflectance over 36 spectral bands between 410 nm and 14 μm at three different spatial resolutions (250 m, 500 m, 1 km) [10].

We obtained the MODIS level-1B2 radiance data product MOD02SSH with spatial resolution of 5 km, covering the 36 AERONET locations between January 2002 and December 2004. Over the same spatial and temporal range, we obtained the level-2 aerosol-retrieval product MOD04 (version 4) with a spatial resolution of 10 km, and level-1B2 radiometric cloud-mask product MOD35 with a resolution of 1 km.

Each MODIS retrieval is given a QA flag, which is an integer between 0 and 3, with 3 being the highest quality and 0 being the lowest. In this letter, retrievals with QA $= 0$ and QA $= 1$ are not used, as their quality is rated as "bad" or "marginal." The aerosol product also provides geometry information such as solar azimuth and zenith angles, sensor azimuth and zenith angles, and scattering angle.

C. Collocated AERONET–MODIS Data

We obtained a total of 3646 spatially and temporally collocated observations from MODIS and AERONET. Consistent with the previous validation studies [11], each observation corresponded to a spatial region of size 30×30 km^2 surrounding an AERONET site, and the observation was generated if the following conditions were met: the region contained at least one noncloud pixel; at least one MODIS AOT retrieval with quality flag QA ≥ 2 was available; and at least one AERONET AOT retrieval was available within 60 min of the satellite overpass.

Each of the 3646 observations was represented as a vector (MODIS_AOT, AERONET_AOT, $\mathbf{x}$), where MODIS_AOT is the average MODIS AOT at 470 nm retrieved by MOD04 operational algorithm within the collocated region, AERONET_AOT is the average interpolated AERONET AOT at 470 nm within 60 min of the satellite overpass, and $\mathbf{x}$ is a 30-D attribute vector. The components of $\mathbf{x}$ are as follows: $(x_1–x_{14})$ are the average and minimum MODIS radiances over cloud-free pixels for seven wavelengths between 0.47–2.1 μm (these wavelengths are also used in the MODIS operational aerosol-retrieval algorithm [12]); $(x_{15}–x_{21})$ are the average MODIS radiance uncertainties for the seven wavelengths over the cloud-free pixels; $(x_{22}–x_{26})$ are the MODIS solar zenith and azimuth angles, sensor zenith and azimuth angles, and scattering angle; (x_{27}) is the fraction of cloud-free pixels; and $(x_{28}–x_{30})$ are the fraction of water, land, and desert pixels among the cloud-free pixels.

III. NN-Based Retrievals

AERONET retrievals were estimated to be up to five times more accurate than MODIS retrievals [5] and can be used as proxies for true AOT values. We constructed NNs that predict AERONET_AOT from the inputs consisting of the 30 MODIS attributes listed earlier. The attributes contain virtually the same information as that used by the MODIS operational algorithm. Such attribute choice allows for an objective comparison between the accuracies of NNs and the MODIS operational algorithm.

To provide retrieval, we used the average prediction from an ensemble of ten feedforward NNs. Each of the ten NNs from the ensemble was trained on examples selected randomly with repetition from the training data [12]. Each neural network had 30 inputs, a single hidden layer with ten sigmoid neurons and a linear neuron at the output. The choice of ten hidden nodes was made based on preliminary studies where this resulted in slightly more accurate networks than when using 5 or 20 hidden nodes. MATLAB implementation of Bayesian regularization backpropagation with default parameters, maximum of 100 epochs, and early stopping (max_fail was set to five) was used in training.

The accuracy of the ensemble was estimated by three-year cross validation; in each of the three rounds of cross validation, an ensemble was trained on two-year data and tested on data from the remaining year. Column 2 of Table I lists the number of observations in each of the three years. The procedure was repeated three times, each time using a different year as the test set; the accuracy reported was an average of the three rounds. Prediction accuracy was calculated as the correlation coefficient (CORR) between AOT predictions and AERONET AOT retrievals and as the root mean square (rms) error.

TABLE I
ACCURACY COMPARISON BY YEAR

Year	#Obs	AOT	MODIS		Refined MODIS		NN Retrieval	
			RMS	CORR	RMS	CORR	RMS	CORR
2002	1271	0.17	0.203	0.80	0.124	0.80	0.111	0.83
2003	1257	0.17	0.195	0.76	0.099	0.76	0.091	0.80
2004	1118	0.15	0.218	0.64	0.111	0.64	0.085	0.75
Total	3646	0.16	0.205	0.74	0112	0.72	0.097	0.80

A. Decision-Tree Analysis of Retrieval Errors

To gain an insight into the performance of the MODIS algorithm, decision trees were used. Decision trees discriminate between positive and negative examples and provide a set of classification rules that are easy to analyze. We performed two types of experiments:

E1) Positives (class c1) are examples where MODIS error was larger than 0.05 while negatives (class c0) are the remaining examples. The resulting tree explains situations where MODIS retrieval error is large.

E2) Positives are examples where the NN was more accurate than MODIS. Considering that both the MODIS algorithm and NNs are using the same set of attributes for retrieval, the resulting tree reveals weaknesses of the MODIS retrieval algorithm that are correctable.

In both experiments, the following attributes were used.

1) Normalized difference vegetation index (NDVI) defined as

$$\mathrm{NDVI} = (\rho_{860} - \rho_{660})/(\rho_{860} + \rho_{660})$$

where ρ_{660} and ρ_{860} are the top-of-atmosphere reflectances at the red band (660 nm) and the near-infrared band (860 nm), respectively.

2) Angstrom exponent (AE) at blue/red wavelength defined as

$$\mathrm{AE} = -\ln(\mathrm{AOT}_{470}/\mathrm{AOT}_{660})/\ln(470/660)$$

where AOT_{470} and AOT_{660} are AERONET AOT at wavelengths 470 and 660 nm, respectively.

3) AERONET AOT at wavelength 470 nm (AOT_{470}).

4) Scattering angle (SA).

IV. RESULTS

A. MODIS Versus Neural Network Retrievals

The accuracies of the MODIS algorithm and NN predictors after the three cross-validation experiments are shown in Table I. Based on the rms error measure, neural networks $(\mathrm{rms} = 0.097)$ were about twice as accurate as the MODIS algorithm $(\mathrm{rms} = 0.205)$. The scatter plot of AERONET AOT versus MODIS AOT shown in Fig. 1(a) reveals a strong bias in the MODIS algorithm that tends to overestimate AOT values. On the other hand, NN predictions appear less biased and tend to underestimate the AOT [Fig. 1(b)].

When measuring the CORR that neglects bias, the overall accuracy of NN predictors $(\mathrm{CORR} = 0.798)$ is about 7% better than that of the MODIS algorithm $(\mathrm{CORR} = 0.743)$. Both rms and CORR results indicate that it should be possible to further improve the MODIS algorithm's accuracy.

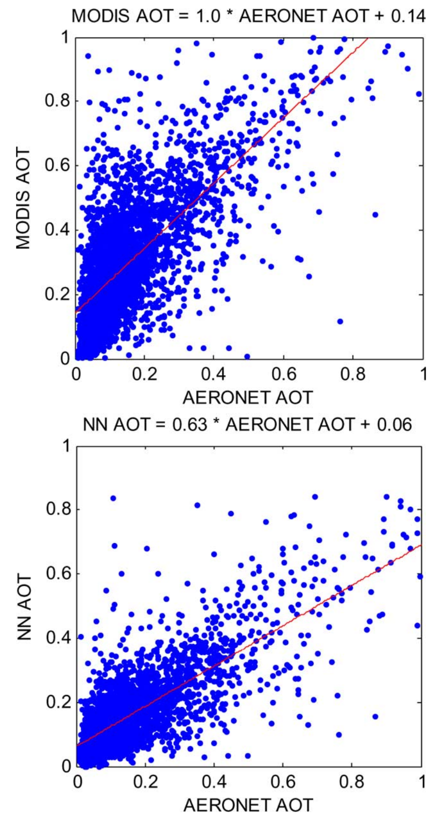

Fig. 1. (a) AERONET AOT versus MODIS AOT. (b) AERONET AOT versus neural network retrieval.

We also explored as to what extent the bias of the MODIS can be removed. Using data from two years, a linear model, $MODIS\_Refined = \alpha_0 + \alpha_1 \cdot MODIS$, was learned and tested on the remaining year. The procedure was repeated three times by reserving year 2002, 2003, and 2004 as a test year; the results are also shown in Table I. The rms of Refined MODIS retrievals was significantly improved $(\mathrm{rms} = 0.112)$, while the CORR was slightly decreased $(\mathrm{CORR} = 0.719)$ as compared to the original MODIS retrieval. However, while the MODIS retrieval accuracy improved, the neural network retrievals were still significantly more accurate.

An analysis of year-by-year fluctuations in the accuracy revealed that the accuracy of both MODIS and neural network algorithms decreased from 2002 to 2004. This is consistent with the recent finding that the MODIS instrument-calibration error increases in time [A. Wu, personal communication]. However, it is interesting to observe that the MODIS-algorithm accuracy decreases more rapidly than that of neural networks, indicating that it is more sensitive to the calibration.

Seasonal variations in prediction accuracy are compared in Table II. The largest difference between the MODIS algorithms and neural networks was observed between January and March, while, in the remaining months, the difference in CORR accuracy was smaller. It is also interesting to observe that the CORR accuracy of both retrieval algorithms was lower during winter months. In comparison, the rms measure indicates a decreased accuracy during the summer months. This phenomenon reflects

TABLE II
ACCURACY COMPARISON BY SEASON

Season	#Obs	AOT	MODIS Retrieval		NN Prediction	
			RMS	CORR	RMS	CORR
Jan-Mar	824	0.107	0.211	0.375	0.084	0.526
Apr-Jun	1234	0.215	0.241	0.759	0.112	0.791
Jul-Sep	755	0.201	0.204	0.820	0.104	0.841
Oct-Dec	833	0.106	0.129	0.626	0.077	0.668

TABLE III
ACCURACY COMPARISON BY LAND TYPE

Surface Type	#Obs	AOT	MODIS Retrieval		NN Prediction	
			RMS	CORR	RMS	CORR
Water	37	0.094	0.446	0.001	0.142	0.098
Coast	52	0.189	0.185	0.909	0.071	0.910
Desert	447	0.100	0.237	0.645	0.069	0.733
Land	2377	0.169	0.196	0.762	0.097	0.809

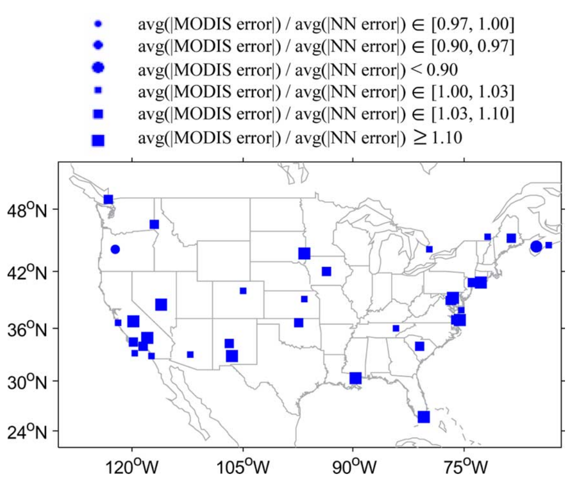

Fig. 2. Comparison between MODIS and NN retrieval errors over 36 AERONET sites.

the fact that AOT values are significantly larger during the summer months.

We then explored the influence of surface types on the retrieval accuracy. In the experiments, a block is classified as a surface-type S if there are more than 30% of valid pixels in the block and more than 50% of such valid pixels have surface-type S. The results in Table III indicate that NNs are the most beneficial over desert surfaces. These results are explained by the increased surface reflection from desert areas. We know from previous studies that the MODIS algorithm is the least successful over bright areas. Our results suggest that, while the retrieval accuracy over desert areas is indeed decreased, it should be possible to further improve the MODIS retrieval accuracy. If the type of surface is water, then neither algorithm performed particularly well. Poor MODIS accuracy might be caused by a less homogenous AOT over the water regions due to more humid environment [13]. In such cases, use of the averaged MODIS AOT could lead to decreased retrieval accuracy. The reason for lower NN retrieval accuracy is probably due to a small number of training data points from water surfaces.

We also compared the MODIS algorithm and NN over each AERONET site (Fig. 2). For each site, we calculated the ratio between the average of absolute MODIS retrieval errors and the average of absolute NN retrieval errors. Neural networks

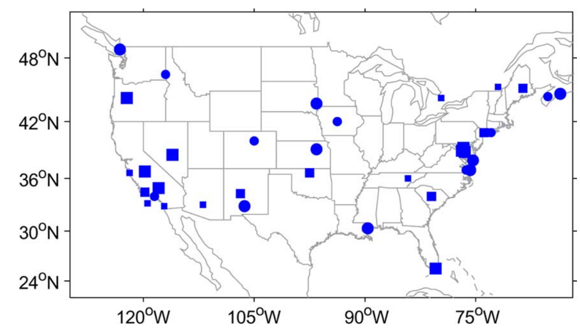

Fig. 3. Comparison between Refined MODIS and NN retrieval errors over 36 AERONET sites.

```
AOT440 <= 0.272
|   SA <= 119
|   |   AOT440 <= 0.204
|   |   |   NDVI <= -0.106: c0 (45/22)
|   |   |   NDVI > -0.106: c0 (736/138)
|   |   AOT440 > 0.204
|   |   |   SA <= 114: c1 (60/21)
|   |   |   SA > 114: c0 (22/6)
|   SA > 119
|   |   NDVI <= 0
|   |   |   SA <= 132: c0 (227/108)
|   |   |   SA > 132: c1 (491/177)
|   |   NDVI > 0: c0 (1433/545)
AOT440 > 0.272
|   AOT440 <= 0.509
|   |   SA <= 147: c1 (270/60)
|   |   SA > 147
|   |   |   NDVI <= 0.345: c0 (124/61)
|   |   |   NDVI > 0.345: c1 (51/11)
|   AOT440 > 0.509: c1 (187/6)
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Fig. 4. First three levels of the decision tree for E1. For example, the underlined tree leaf corresponds to examples where $\texttt{AOT}_{440} <= 0.272$ AND SA > 119 AND NDVI > 0. There are 1433 of such examples, majority of them are negative (c0), and 545 of them are from the minority (i.e., positive) class.

were more accurate for almost all sites (34 of 36). In a similar comparison of Refined MODIS versus NNs (Fig. 3), retrievals in 15 of the 36 AERONET sites the Refined MODIS algorithm was more accurate. Form Fig. 3, it can be observed that location has significant impact on the retrieval-error differences—NNs are superior in the southwest, while the MODIS algorithm is more successful in the northeast coastal region.

B. Decision-Tree Analysis of Retrieval Errors

The C4.5 decision-tree algorithm with the default parameters as implemented in the open-source software Weka (J48) was used to construct the decision trees. Tenfold cross validation was used to estimate their accuracy. The tree for E1 (high/low MODIS error) had accuracy of 66.5%, which was above the majority prediction accuracy of 53.6% (the fraction of positives). The tree for E2 (MODIS less/more accurate than neural network) had accuracy of 59.5%, which was above the majority prediction accuracy of 54.4% (the fraction of positives). This result indicates that it is possible to gain a partial understanding of the differences between positive and negative examples in both experiments.

In Figs. 4 and 5, we show the initial portion (the first three levels) of the resulting decision trees. An analysis of the decision tree from Fig. 4 reveals conditions when the refined MODIS retrieval results in errors larger than 0.05. When

```
NDVI <= 0
|   SA <= 113: c0 (251/118)
|   SA > 113
|   |   AOT440 <= 0.154
|   |   |   NDVI <= -0.275: c0 (20/7)
|   |   |   NDVI > -0.275: c1 (623/160)
|   |   AOT440 > 0.154: c0 (198/94)
NDVI > 0
|   AOT440 <= 0.0675
|   |   SA <= 148: c0 (410/125)
|   |   SA > 148: c1 (36/15)
|   AOT440 > 0.0675
|   |   AOT440 <= 0.285
|   |   |   NDVI <= 0.207: c1 (893/396)
|   |   |   NDVI > 0.207: c0 (704/297)
|   |   AOT440 > 0.285: c1 (511/179)
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Fig. 5. First three levels of the decision tree for E2.

$\text{AOT}_{440} > 0.272$, a majority of retrievals have significant errors, and this is particularly the case when $\text{AOT}_{440} > 0.509$. This result is consistent with the well-known findings that retrieval uncertainty is larger at large aerosol loadings. This is an inherent property of aerosol retrieval and is an example of noncorrectable retrieval error. NDVI < 0 is corresponding to cases that might be contaminated by cloud, or the surface is snow or water. When the AOT is small $(\text{AOT}_{440} < 0.272)$ and the NDVI is negative, the error of MODIS retrieval is more difficult to correct. This is particularly the case when the scattering angle is large $(\text{SA} > 132)$ because the algorithm is limited by cloud, snow, or water contaminations [14].

An analysis of the decision tree from Fig. 5 reveals conditions where the Refined MODIS retrievals are less accurate than NN retrievals. Understanding the conditions behind such accuracy results reveals the sources of correctable retrieval errors. The decreased classification accuracy of the E2 tree (at 59.5%) as compared to the E1 tree (at 66.5%) is expected and confirms that it is more difficult to understand the sources of correctable errors than to grasp the situations that ultimately lead to large errors.

Apparently, NNs are generally more accurate than refined MODIS when the retrieval is contaminated by clouds, snow, or water (i.e., NDVI $<= 0$). When aerosol loading is small $(\text{AOT} <= 0.258)$ and the surface has less vegetation $(\text{NDVI} <= 0.207)$, then the inaccurate surface-reflectance assumptions in the MODIS algorithm dominate and induce a significant error to the total AOT retrieval. In addition, MODIS tends to underestimate AOT when aerosol loading is large $(\text{AOT} >= 0.285)$ because the uncertainties of assumed aerosol model dominate. This is consistent with most global studies [5], [9]. On the other hand, the quality of MODIS retrieval is not sensitive to aerosol particle size, since the AE plays a less important role in the decision tree (decisions involving AE do not appear in Fig. 5; however, there were several decisions involving AE that occurred deeper in the tree).

V. Conclusion

We proposed a data-mining method to help aerosol scientists with the improvement of the MODIS operational retrieval algorithm. The results over the continental U.S. during the periods between 2002 and 2004 indicate that the MODIS aerosol-retrieval accuracy could be significantly improved. Decision-tree analysis indicates that conditions that present the biggest opportunity for the operational algorithm improvement are characterized by cloud contamination, high aerosol loading, and the presence of bright surfaces. While this letter focused on aerosol retrieval, it is evident that the proposed approach is directly applicable to similar remote-sensing problems.

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