Identifying Aerosol Type from Space: Absorption Wavelength Dependence as a Foundation for Multidimensional Specified Clustering and Mahalanobis Classification Phil Russell* & the Glory Aerosol ClassificationTeam[#]

*NASA Ames Research Center #SJSU, SRI, BAER, NASA LaRC, NASA GISS, U. Hawaii, ...



LOA-CNES Workshop on Aerosol & Cloud Properties for Climate Studies, Paris, FR, Sep 2011



Identifying Aerosol Type from Space:

Absorption Wavelength Dependence as a Foundation for Multidimensional Specified Clustering and Mahalanobis Classification

The Glory Aerosol Classification Team

Phil Russell NASA Ames Research Center

Patrick Hamill San Jose State University

> John Livingston SRI International

Yohei Shinozuka, Jens Redemann, and Robert Bergstrom Bay Area Environmental Research Institute

> Ali Omar, Richard Ferrare and Sharon Burton NASA Langley Research Center

> > Antony Clarke University of Hawaii

Brent Holben NASA Goddard Space Flight Center

Kirk Knobelspiesse and Brian Cairns NASA Goddard Institute for Space Studies



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Goal of this work:

Identify aerosol type using only the opto-physical* information retrieved from a single data grid box*

*But the algorithm can be trained using other information (e.g., trajectories, accompanying trace gases, ...)



LOA-CNES Workshop on Aerosol & Cloud Properties for Climate Studies, Paris, FR, Sep 2011

Sahara dust

Wildfire

smoke

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Suggests that knowledge of AAE can help identify aerosol type

Black Carbon: AAE = 1

[Russell et al., ACP 2010]



- This holds out the promise of determining aerosol composition from <u>space</u>, <u>provided Absorption</u> <u>Angstrom Exponent can be determined from space</u>.

1F. The A-Train with Glory



Glory Aerosol Polarimetry Sensor (APS) level-3 data products for aerosol columns

(adapted from Mishchenko et al., 2007)

Data product (fine and coarse modes)	Range	Uncertainty	Absorption
Spectral* aerosol optical depth	0-5	0.02 over ocean	
		0.04 over land	
Aerosol effective radius	0.05-5 μm	10%	[
Effective variance of aerosol size	0-3	40%	$\wedge \wedge \cap D =$
distribution			
Aerosol spectral* real refractive index	1.3-1.7	0.02	
Aerosol spectral* single-scattering albedo	0-1	0.03	AUD"(1-55A
Aerosol morphology	Spherical aerosols, irregular	N/A	▲ · ·
	dust particles, soot clusters		
*At least in three spectral channels: relative accu	tracy better where AOD is larger (typ	nically 410-865 nm).	•

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Lost on launch, Mar 2011

Possible refly.Airborne version:

- Others: POLDER, PACE, ACE, ...



RSP

Question: Do the preceding results, which describe a <u>layer</u> or a <u>point</u>, apply also to the <u>full vertical</u> <u>column</u> viewed by a spacecraft?



To answer, we looked at many <u>full vertical</u> <u>columns</u> as viewed by AERONET sun-sky photometers (Dubovik et al., 2002)



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Question: Can we get more separation between types by adding a second parameter and making a 2-D plot?



Answers: 1. Adding EAE(440, 870 nm) greatly increases separation between Dust and the others.

2. But it increases separation between the UrbInd & BioBurn clusters only slightly: There is still overlap (ambiguity).

Question: Can we do better by adding more parameters (dimensions)?

2D. Different 2-D plots of Dubovik (2002) AERONET fullcolumn results, showing different separations of clusters



Questions:

1.Can combining all 3 dimensions (AAE, EAE, RRI) produce even better separation between types?

2.Can adding still <u>more dimensions (e.g., SSA, imaginary refractive index</u> [IRI], ..., additional λ) improve separation further?

3.Given an individual aerosol observation (point in multidimensional space), is there an objective, quantitative way to measure the multidimensional distance from that point to a cluster (or type)?

- And hence <u>decide objectively which cluster (aerosol type) the</u> observation best matches?

4. Do the preceding results for the Dubovik et al. (2002) data (AERONET Version 1, site/season means) carry over to individual AERONET retrievals using the Version 2 algorithm?

To answer the above, we followed the example provided by the <u>HSRL aerosol classification technique (Burton et al., AMTD 2011)</u> and used <u>Specified Clustering</u> and <u>Mahalanobis Classification</u>

Specified Clustering and Mahalanobis Classification



<u>Mahalanobis Distance, D_M:</u>

The distance between an <u>observation</u> [n-dimensional vector $\mathbf{x}=(x_1,x_2,...,x_n)$] and a <u>cluster</u>, taking into account the <u>standard deviations</u> and <u>cross-</u> <u>correlations</u> of the cluster.



Mahalanobis Classification:

Assigns an observation to the class (cluster) from which it has least D_M . This is also the class for which it has the highest probability density

$$f(D_M) = K \exp\left\{-\frac{D_M^2}{2}\right\}.$$

4 AERONET sites/seasons from Cattrall et al. (*JGR*, 2005) selected to illustrate specified clustering and Mahalanobis classification



Different 2-D plots of Dubovik (2002) AERONET fullcolumn results, showing different separations of clusters



Classification Boundaries and Skill* Scores



*More accurately, "Sameness Scores"

At λ =870 nm, Skill* Scores have increased to 93%



*More accurately, "Sameness Scores"



Are these cases of wildfire smoke over GSFC, like the image at right?



Black "x"s: Mahal. Class. saying a point measured at GSFC is more like BioBurn than a typical day at GSFC



Coordinates other than AAE: SSA(441 nm) vs EAE(440,870 nm)



19-Jul-2011 09:56:01 Calcplot-Mahal-for-Cattrall-Aeronet-V09.m

Skill* scores 95% to 99%



*More accurately, "Sameness Scores"

07-Dec-2010 17:14:07 Calcplot-Mahal-for-Cattrall-Aeronet-V08.m

5-D Mahalanobis classification of Bahrain data assigns 89% of Bahrain points to the Solar Village (Dust) cluster and 11% to the Beijing (AsiaUrb) cluster.





Aerosol models as a path to simulation of Glory APS products



Models used in MODIS retrievals combine a fine mode and a coarse mode (e.g., Remer et al., 2005). Diamonds below show SSA-EAE coordinates of MODIS over-ocean set (modes 1-9), augmented with increased absorption (modes 10-18) and adjusted size (modes 19, 20). Together the lines cover the SSA, EAE space of the AERONET clusters from the 4 Cattrall sites.



1F. The A-Train with Glory



Glory Aerosol Polarimetry Sensor (APS) level-3 data products for aerosol columns

(adapted from Mishchenko et al., 2007)

Data product (fine and coarse modes)	Range	Uncertainty
Spectral* aerosol optical depth	0-5	0.02 over ocean
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Aerosol morphology	Spherical aerosols, irregular	N/A
	dust particles, soot clusters	

Uncertainties used in simulations

*At least in three spectral channels; relative accuracy better where AOD is larger (typically 410-865 nm).



Simulated measurements and classifications: Skill scores 71-99%



Boundaries: from the Cattrall-site

clusters

Mahalanobis classification using those boundaries produces skill scores 71-99%. Points classified as "unknown" have $D_M>3$ (P(D_M) <1%) for all 4 Cattrall-based clusters.

Summary and Conclusions

 Increasingly, aerosol remote sensors (e.g., Glory, RSP, POLDER...) produce <u>multidimensional</u> retrieved aerosol properties [e.g., EAE(λ₁, λ₂), AAE(λ₁, λ₂), SSA(λ₁,...,λ_n), RRI
 RRI(λ₁,...,λ_n), IRI(λ₁,...,λ_n), several size parameters, shape]—like AERONET.



- AERONET.
 Specified clustering and Mahalanobis classification together provide a useful way of <u>combining several dimensions</u> of multiwavelength optical
- information to <u>assign aerosols to classes</u> (e.g., Urban-Industrial, Biomass-Burning, Mineral Dust, Asian Urban, …).
- The specified or <u>"reference" clusters</u> can be established using information (e.g., trajectories, accompanying trace gases, chemical analyses, prior studies) <u>beyond the optical information that will be</u> <u>available in the general case</u>. These reference clusters can then be used to <u>train and test</u> the classification algorithm.
- <u>Applications</u> of the technique to <u>2 AERONET data sets</u> and <u>aircraft-sampled aerosols</u> yielded <u>skill* scores ranging from 87% to 100%</u> (diagonal elements of the skill score matrix).
- *More accurately, "sameness scores"

Summary and Conclusions (cont'd)



A first step toward <u>simulating Glory APS data</u>, by using bimodal aerosol <u>models with randomly generated errors</u> based on Glory APS expected uncertainties, yielded <u>skill scores of 71% to 99%</u>, with 0% to 12% of simulated points assigned to an "unknown" class (defined as consisting of points with D_{Mahal}>3 from all 4 reference clusters based on 4 AERONET sites and associated seasons).

<u>Next Steps</u>

- Begin to apply technique to other multidimensional data sets beside AERONET:
 - RSP (airborne Glory APS)
 - RSP + HSRLidar
 - POLDER (Dubovik et al. AMT 2011)
 - 4STAR* (sun-sky spectrometer: more in Redemann talk later this morning)

*Spectrometer for Sky-Scanning Sun-Tracking Atmospheric Research











End of Presentation

Remaining slides are backup

Separation also good using Imaginary Refractive Index— Skill Scores 95% and 99%



Similar result from very different methods in situ sampling on C-130 over Mexico



Shinozuka, Clarke, DeCarlo, Jimenez in Russell et al., ACP 2010

Specified clustering and Mahalanobis classification can also be applied to in situ data:

Aircraft-sampled aerosols [Clarke et al., JGR 2007]



4 AERONET sites/seasons from Cattrall et al. (*JGR*, 2005) selected to illustrate specified clustering and Mahalanobis classification



Since Dust and AsiaUrb are well separated from BioBurn and UrbInd in AAE-vs-EAE, we can use these 2 dimensions to eliminate them and focus on separating BioBurn and UrbInd from each other.





AERONET sites and months from Cattrall et al. (*JGR*, 2005) selected to illustrate specified clustering and Mahalanobis classification

Site Name	Country	Cattrall	Months*	Years [#]	N _{meas}	
		nation			Raw	Filtered [D _M ≤3]
GSFC	USA	UrbInd	Jun-Sep	1992-200 9	817	802
Mongu	Zambia	BioBurn	Aug- Nov	1995-200 8	1513	1490
Beijing	China	AsiaUrb	Jun-Feb	2000-200 9	1538	1489
Solar Village	Saudi Arabia	Dust	Mar-Jul	1999-200 8	1573	1513

*Designated by Cattrall et al. #Used by our analyses.



Do the individual, Version 2 retrievals from Cattrall (2005) sites/seasons give results like this from the Dubovik (2002) Version 1 site/season means?

Extending to shorter λ (e.g., the OMI λ range) could help increase differences between UrbInd & BioBurn









OMI λ range (343-484 nm) extends into a region where absorption by organics is strongest.

This may increase distinction between BioBurn & UrbInd classes.



Question: Do the preceding results, which describe a <u>layer</u> or a <u>point</u>, apply also to the <u>full vertical column</u> viewed by a spacecraft?

To answer, we looked at many <u>full vertical columns</u> as viewed by AERONET sun-sky photometers (Dubovik et al., 2002)



Background on Radiative Flux Divergence & Closure, Absorption Spectra, etc. **Downwelling Flux: F** 2000_m **Upwelling Flux: F**[↑] Net Flux: F↓- F↑ Flux Divergence (absorption): $(F\downarrow - F\uparrow)_{2000m} - (F\downarrow - F\uparrow)_{43m}$ **Fractional absorption:** $[(\mathsf{F} \downarrow - \mathsf{F} \uparrow)_{2000m} - (\mathsf{F} \downarrow - \mathsf{F} \uparrow)_{43m}]/\mathsf{F} \downarrow_{2000m}$ **43 m Solar Spectral** SOLAR SPECTRAL FLUX RADIONETER **Flux Radiometer** F↓, F↑ (SSFR) **Pilewskie & Gore,** NASA Ames



Pilewskie, Bergstrom, Schmid et al.

Aerosol Single Scattering Albedo Spectrum





Derived from measured flux and AOD spectra.

Desirable features:

- Describes aerosol in its ambient state (incl volatiles like water, organics, nitrates)
- Wide λ range: UV-Vis-SWIR

• Includes λ range of OMI-UV, OMI-MW, MISR, MODIS, CALIPSO, HSRL, Glory ASP, RSP, POLDER,

• Coalbedo (1-SSA) varies by factor 4, λ = 350-900 nm

. . .

 [Bergstrom, Pilewskie, Schmid et al., JGR 2004]

P. Russell, NASA Ames Director's Colloquium, 23 Jun 2009



Wavelength, nm

Bergstrom et al., ACP, 2007

Aerosol <u>Absorption</u> Optical Depth (AAOD) Spectra from 5 Experiments



Aerosol Single Scattering Albedo Spectrum



P. Russell, NASA Ames Director's Colloquium, 23 Jun 2009

4 AERONET sites/seasons from Cattrall et al. (*JGR*, 2005) selected to illustrate specified clustering and Mahalanobis classification



18-Jul-2011 17:17:12 Calcplot-Mahal-for-Cattrall-Aeronet-V09.m

All Cattrall Sites





Coordinates other than AAE: SSA(441 nm) vs EAE(440,870 nm)



18-Jul-2011 17:05:26 Calcplot-Mahal-for-Cattrall-Aeronet-V09.m

All Cattrall Sites



Question: Do the preceding results, which describe a layer or a point, apply also to the full vertical column viewed by a spacecraft?



AERONET Version 2, building on Cattrall et al. (2005)



Mahalanobis Characterization of AERONET data, Cattrall Sites - 2D: eae:1 aae:0 ssa:1 rri:0 iri:0 GSFCdata, Solardata, Mongudata, Beijingdata



⁰⁷⁻Dec-2010 17:14:07 Calcplot-Mahal-for-Cattrall-Aeronet-V08.m

4.3A. 2-D Mahalanobis classification for 4 Cattrall sites



Mahalanobis Characterization of AERONET data, Cattrall Sites - 2D: eae:1 aae:0 ssa:1 rri:0 iri:0 GSFCdata, Solardata, Mongudata, Beijingdata



07-Dec-2010 17:14:07 Calcplot-Mahal-for-Cattrall-Aeronet-V08.m

Meet the family...



And what we do with these beautiful instruments...





4STAR: Spectrometer for Sky-Scanning, Sun-Tracking

Atmospheric Research

AERONET-like

Phase function
 Size mode distributions

- n_{re}(λ), n_{im}(λ)
- Single-scattering albedo
- Asymmetry parameter
- Shape
- Hence aerosol type







Improve H₂O, O₃ Add NO₂ Thus improve AOD

Simultaneous spectra yield airborne profiles of aerosol type via Aeronet-like retrievals AATS-14 like retrievals of column amount and profiles of aerosol, H₂O and O₃

Spectrometer for Sky-Scanning, Sun-Tracking Atmospheric Research (4STAR)



4STAR Integration on PNNL/Battelle G-1 Aug-Sep 2010



4STAR Test flights on PNNL/Battelle G-1 Sep 2010





3 flights:

1.Pilots only: Airworthiness certification 2.Science ops: Pasco, WA to San Jose, CA 3.Science ops: San Jose local Flights met all goals (sun tracking only). Large data set to guide improvements & test/demo flights in 2011.



Pacific Northwest

Skill* Scores



Skill Score Matrix

Mahal.	Cattrall designation							
desig.	Urb	olnd	Du	ust	BE	Burn	Asi	iaUrb
Urbind: o	763	95%	0	0%	9	1%	23	2%
Dust: +	0	0%	1502	99%	0	0%	8	1%
BBurn: *	14	2%	0	0%	1445	97%	1	0%
AsiaUrb: +	25	3%	11	1%	36	2%	1457	98%
Total	802	100%	1513	100%	1490	100%	1489	100%



The A-Train with Glory



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(adapted from Mishchenko et al., 2007)

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Lost on launch, Mar 2011

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RSP

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Aerosol morphology	Spherical aerosols, irregular	N/A	
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02-Aug-2011 12:03:06 Calcplot-Mahal-for-Cattrall-Aeronet-V09.m

For RRI, separation increases with λ , and so do Skill Scores







- **Significance:** Both the radiometric and the in situ results indicate that knowledge of Absorption Angstrom Exponent, plus size (or Extinction or Scattering Angstrom Exponent) can help to determine particle composition.
- This holds out the promise of determining aerosol composition from space, provided Absorption Angstrom Exponent can be determined from space.
- Glory APS promised to do this. The airborne version, RSP, continues to do so.

Next Steps



AERONET:

h airborne <u>RSP data</u>

RONET sites and and the <u>generality of</u> —the news is good!]

 Extend input data sets to parameters non-other sensors (e.g., CALIOP layer heights, OMI UV absorption).

- Begin to apply techr
 RSP
 - RSP + HSRL
 - POLDER (Dubovik
 - 4STAR
- Improve realism of Glo and also <u>enhanced I</u>
- <u>Extend tests</u> to more retrieved parameters <u>aerosol type assigni</u>

