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# A comparison of error metrics and constraints for multiple endmember spectral mixture analysis and spectral angle mapper

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#### Abstract

Spectral matching algorithms can be used for the identification of unknown spectra based on a measure of similarity with one or more known spectra. Two popular spectral matching algorithms use different error metrics and constraints to determine the existence of a spectral match. Multiple endmember spectral mixture analysis (MESMA) is a linear mixing model that uses a root mean square error (RMSE) error metric. Spectral angle mapper (SAM) compares two spectra using a spectral angle error metric. This paper compares two endmember MESMA and SAM using a spectral library containing six land cover classes. RMSE and spectral angle for models within each land cover class were directly compared. The dependence of RMSE on the albedo of the modeled spectrum was also explored. RMSE and spectral angle were found to be closely related, although not equivalent, due to variations in the albedo of the modeled spectra. Error constraints applied to both models resulted in large differences in the number of spectral matches. Using MESMA, the number of spectra modeled within the error constraint increased as the albedo of the modeled spectral matching algorithm. © 2004 Published by Elsevier Inc.

Keywords: Error metrics; Constraints; Spectral mixture analysis; Spectral angle mapper

# 1. Introduction

Spectral matching algorithms allow the identification of an unknown spectrum using one or more reference spectra. Two spectral matching algorithms, multiple endmember spectral mixture analysis (MESMA; Roberts et al., 1998) and spectral angle mapping (SAM; Kruse et al., 1993) have found widespread acceptance in the remote sensing community for determination of spectral similarity. MESMA and SAM have been used for a wide array of applications. MESMA has been extensively used for mapping vegetation species in Southern California chaparral (Roberts et al., 1998; Dennison & Roberts, 2003a). MESMA has also been used to map snow grain size (Painter et al., 1998, 2003), lunar surface composition (Li & Mustard, 2003) and vegetation and soils in semi-arid environments in California (Okin et al., 2001). SAM has been applied to a similar range of applications, including mineral identification (Kruse et al., 2003), monitoring land cover change (Sohn et al., 1999), and discrimination of vegetation type (Lass et al., 2002; Silvestri et al., 2003). Although MESMA and SAM are widely used, the decision of which spectral matching algorithm to use is often based on experience and available software implementation. The intrinsic assumptions and abilities of each spectral matching algorithm may have a discernable impact on model results. This paper explores similarities and differences in the error metrics and error constraints used by MESMA and SAM.

#### 2. Background

MESMA models spectra as a linear mixture of two or more "endmember" spectra, and is based on spectral mixture

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analysis (SMA; Adams et al., 1993). SMA techniques typically utilize a "shade" endmember that is used to account for variations in spectral albedo, while one or more non-shade endmembers can be used to identify the spectral constituents of the modeled spectrum (Smith et al., 1990). Each endmember is assigned a fractional abundance, such that the reflectance of a modeled spectrum ( $\rho'_{\lambda}$ ) is determined by the sum of the reflectance of each material within a pixel multiplied by its fractional cover:

$$\rho_{\lambda}' = \sum_{i=1}^{N} f_i^* \rho_{i\lambda} + \varepsilon_{\lambda} \tag{1}$$

where  $\rho_{i\lambda}$  is the reflectance of endmember *i* for a specific band  $(\lambda)$ ,  $f_i$  is the fraction of the endmember, and *N* is the number of endmembers. The fit of the model is assessed by an error metric based on  $\varepsilon_{\lambda}$ , the residual error. Since the residual error is not scaled by the endmember fractions,  $\varepsilon_{\lambda}$  increases with an increase in the reflectance of the modeled spectrum.

MESMA uses the SMA linear model, but rather than using a rigid set of endmembers, MESMA allows endmembers to vary on a per-pixel basis (Roberts et al., 1998). The two-endmember case of MESMA can be used for spectral matching (Roberts et al., 1998; Dennison & Roberts, 2003a). The standard error metric for MESMA is root mean square error (RMSE; Roberts et al., 1998). RMSE is calculated as:

$$RMSE = \sqrt{\frac{\sum_{\lambda=1}^{M} (\varepsilon_{\lambda})^2}{M}}$$
(2)

where M is the number of bands. Since the residual error is partially dependent on the reflectance of each band within the modeled spectrum, RMSE will be partially dependent on the albedo of the modeled spectrum. As the albedo of the modeled spectrum increases, RMSE will also increase.

SAM resolves spectral similarity by calculating a spectral angle between two spectral vectors that have a common origin. The length of a spectrum vector  $(L_{\rho})$  is calculated as:

$$L_{\rho} = \sqrt{\sum_{\lambda=1}^{M} \rho_{\lambda}^2} \tag{3}$$

The spectral angle  $(\theta)$  is calculated as:

$$\theta = \cos^{-1} \left( \frac{\sum_{\lambda=1}^{M} \rho_{\lambda} \rho_{\lambda}'}{L_{\rho} L_{\rho'}} \right)$$
(4)

where  $L_{\rho}$  is the length of the endmember vector and  $L_{\rho'}$  is the length of the modeled spectrum vector calculated using Eq. (3) (Kruse et al., 1993). Spectral angle itself is the error metric for SAM. If the spectral angle of a modeled spectrum is below a user-determined threshold, the spectrum is classified as belonging to the endmember class. One of the primary advantages of SAM is that spectral angle is insensitive to differences in the albedo of the modeled spectrum. Spectral angle only measures differences in spectral shape, and spectral albedo is measured by the length of each vector.

Schwarz and Staenz (2001) describe a two step process for determining spectral similarity. First, an error metric is calculated for the algorithm being used. Second, an error constraint is used to determine whether spectral similarity is present or not. Error constraints are typically selected to minimize classification errors, although automated means of selecting error constraints have been proposed (Schwarz & Staenz, 2001).

Fig. 1 illustrates how error constraints differ for MESMA and SMA. An endmember (A) is used to model a spectrum (B), both of which are displayed as vectors with reflectance components from two spectral bands. RMSE (solid lines) and spectral angle (dashed line) error metrics are shown. For MESMA, B is modeled as a linear mixture of A and photometric shade, represented by the origin. A RMSE constraint is shown as the shaded area (Fig. 1). A spectral match is found if the RMSE is within the shaded area. The albedo of A can change, allowing the endmember to slide to any point along the vector, but the albedo of B is fixed. The RMSE error constraint is parallel to the endmember vector, since the shortest distance (lowest RMSE) from the endmember vector to a point along the modeled spectrum vector is a line perpendicular to the endmember vector. If the modeled spectrum is dark  $(B_1)$ , then RMSE will be small and may fall below the specified error constraint (Fig. 1). If the modeled spectrum is bright  $(B_2)$ , RMSE will be larger and may exceed the error constraint. For SAM, the albedo of the modeled spectrum does not matter with respect a



Fig. 1. Two spectra, endmember A and modeled spectrum B, are shown plotted as a vectors with reflectance components from two spectral bands. f represents the fraction of endmember A. The distance from the origin indicates the albedo of each point along the vectors. RMSE and spectral angle error metrics are indicated by the solid and dashed lines, respectively. A RMSE error constraint is represented by the shaded area. The RMSE constraint to the left of endmember A has been omitted for the purpose of clarity.

spectral angle error constraint. The spectral angle between A and B will be the same for any pair of points along A and B. For  $f_1A$  and  $B_1$ , the spectral angle will be equivalent to a smaller RMSE, while for  $f_2A$  and  $B_2$ , the spectral angle will be equivalent to a larger RMSE. Over the entire range of albedos, there is no direct equivalence between RMSE and spectral angle error constraints.

## 3. Methods

#### 3.1. Spectral Library

A library containing 988 spectra of six land cover types was used to compare error metrics and error constraints from MESMA and SAM (Table 1). The library spectra were extracted from a June 14, 2001 Airborne Visible Infrared Imaging Spectrometer (AVIRIS) scene covering the city of Santa Barbara and the south-facing slope of the Santa Ynez Mountains, in California, USA. AVIRIS is a 224 band imaging spectrometer that covers a spectral range from 400 to 2500 nm (Green et al., 1998). The instrument was flown on the high altitude ER-2 platform, producing an image swath width of approximately 11 km and an instantaneous field of view of approximately 20 m. AVIRIS radiance data were processed to apparent surface reflectance using a modified version of the MODTRAN radiative transfer model (Green et al., 1993). Reflectance was subsequently adjusted using a field measured spectrum of a sand target (Clark et al., 2002). The reflectance corrected AVIRIS scene was registered to an orthorectified SPOT mosaic, transformed using triangulation and resampled using nearestneighbor resampling. A subset of 174 bands from the registered reflectance image was selected to remove bands with strong water absorption features in the shortwave infrared (SWIR) and bands with poor signal-to-noise in the blue end of the visible spectrum and the SWIR beyond 2450 nm wavelength.

Reflectance spectra were extracted from the AVIRIS image from fifty-nine reference polygons that were at least 75% dominated by a single land cover type (Dennison & Roberts, 2003b). The six land cover classes are listed in

Table 1

Description of the six	land co	over classes	in the	spectral	library
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Land cover class	Scientific name	Abbreviation	Number of spectra
Chamise	Adenostoma fasciculatum	adfa	77
Manzanita	Arctostaphylos spp.	argl	111
Big pod ceanothus	Ceanothus megacarpus	ceme	398
Grassland	multiple	gras	116
Coast live oak	Quercus agrifolia	quag	107
Impervious surf.	N/A	impv	202

Table 1. Polygons for the five vegetation classes (*Adenostoma fasciculatum*, *Arctostaphylos* spp., *Ceanothus megacarpus*, *Quercus agrifolia*, and mixed introduced grasses) were mapped in June 2002 using field assessed vegetation cover and a 1-m resolution United States Geological Survery Digital Orthophoto Quadrangle (DOQ). A sixth class, impervious surface, was mapped using the DOQ in January 2003. Polygons were required to be at least 40 m by 40 m in size, and only spectra that were entirely inside a polygons were extracted to reduce potential spectral mixing and the effects of registration errors (Dennison & Roberts, 2003b). The polygons contained between two and seventy-two image spectra, with a mean of 16.8 spectra per polygon.

### 3.2. Spectral modeling

Two endmember MESMA and SAM were used to model combinations of spectra from the spectral library. The library was subset by land cover class, and each spectrum within a class was used to model the members of the class. The total number of models  $(n_m)$  can be calculated as:

$$n_{\rm m} = n_{\rm s}^2 - n_{\rm s} \tag{5}$$

where  $n_s$  is the number of spectra in the class, and each spectrum modeling itself is excluded from the total number of models. If fractional constraints are not imposed, the error matrix is symmetric and the number of unique models in each class becomes

$$n_{\rm m} = \frac{n_{\rm s}^2 - n_{\rm s}}{2} \tag{6}$$

Several of the classes were sufficiently large enough that displaying model parameters became difficult, so each class was subset. Fifty spectra were randomly selected from each land cover class, creating 2450 model pairings and 1225 unique models for each land cover class.

Three different types of comparisons between MESMA and SAM were investigated:

- 1. comparison of MESMA and SAM error metrics for all model pairings within a land cover class,
- comparison of the number of spectra modeled by a selected endmember within set MESMA and SAM error constraints, and
- comparison of the MESMA and SAM error metrics for spectra modeled by a selected endmember, across all six land cover classes.

Two endmember MESMA and SAM were used to model each spectral pairing within each land cover class. For each model pairing, one spectrum was designated as the "endmember" and a second spectrum was designated as the "modeled spectrum". In the case of MESMA, a photometric shade endmember with a uniform reflectance of zero was also used. MESMA was not constrained by fractional or residual constraints. For MESMA, the RMSE



Fig. 2. Spectral angle vs. RMSE for six land cover types.

and endmember fractions were calculated for each model using singular value decomposition to solve Eq. (1) (Boardman, 1989). For SAM, the spectral angle was calculated using Eq. (4). The lengths of the endmember spectrum vector  $(L_{\rho})$  and the modeled spectrum vector  $(L_{\rho'})$  were calculated using Eq. (3).

Error metrics for MESMA and SAM were compared for each land cover class using linear regression. RMSE was modeled as a function of spectral angle, and the resulting slope and intercept terms were used to calculate RMSE residuals. RMSE residuals were then compared to the vector lengths of the modeled spectra to examine the effects of albedo on MESMA.

The effects of error constraints on spectral matching using MESMA and SAM were also examined. A single endmember was selected for each land cover class using Endmember Average RMSE (EAR). EAR is the average RMSE for an

endmember modeling its own spectral class using MESMA (Dennison & Roberts, 2003a). EAR is calculated as:

$$EAR_{A_i,B} = \frac{\sum_{j=1}^{n} RMSE_{A_i,B_j}}{n-1}$$
(7)

where A is the endmember class,  $A_i$  is the endmember, B is the modeled spectra class, and n is the number of modeled spectra in class B. The "n-1" term accounts for the endmember modeling itself. An equivalent endmember selection method can be created for SAM. The average spectral angle for an endmember modeling its own class using SAM can be calculated as:

$$\bar{\theta}_{A_i,B} = \frac{\sum_{j=1}^n \theta_{A_i,B_j}}{n-1} \tag{8}$$

Table 2 Slope, intercept, and  $R^2$  for linear regressions of spectral angle (in radians) against RMSE

Land cover class	Slope	Intercept	$R^2$
	(RMSE /0/SA)	(KWBE 70)	
Chamise	22.3	-0.066	0.987
Manzanita	20.5	-0.026	0.984
Big pod ceanothus	19.6	-0.015	0.994
Grassland	22.9	0.065	0.966
Coast live oak	20.1	0.022	0.994
Impervious surf.	22.8	0.015	0.865

Endmembers selected using minimum EAR and minimum average spectral angle techniques were compared.

The EAR-selected endmembers were used to model their individual land cover classes using MESMA and SAM. A set of five error constraints for MESMA (2.5, 2.0, 1.5, 1.0, and 0.5 RMSE, in percent reflectance) and four error constraints

Table 3 Number of spectra modeled by MESMA within a given constraint for each land cover class

Constraint	Number of spectra modeled						
	adfa	argl	ceme	gras	quag	impv	
0.5%	11	14	5	12	14	1	
1.0%	28	31	27	31	36	16	
1.5%	35	42	39	37	40	39	
2.0%	38	45	46	41	42	45	
2.5%	43	49	47	43	44	50	

for SAM (spectral angles of 0.2, 0.15, 0.1, and 0.05, in radians) were used to determine the number of spectra modeled in each land cover class at or below each constraint. Error constraints were selected arbitrarily, and should not be used as evidence of better performance of one model over another. Since MESMA was shown to be sensitive to the albedo of the modeled spectrum, the albedos of the modeled



Fig. 3. Vector length of the modeled spectra vs. RMSE residuals for each land cover class.

Table 4 Number of spectra modeled by SAM within a given constraint for each land cover class

Constraint (radians)	Numb	Number of spectra modeled					
	adfa	argl	ceme	gras	quag	impv	
0.05	30	30	26	33	36	23	
0.1	40	45	46	42	42	49	
0.15	46	50	49	46	45	50	
0.2	48	50	50	48	47	50	

spectra were also scaled by a multiplier. Twenty albedo multipliers ranging from 1.0 (no change in albedo from the original spectrum) to 0.05 (5% of the original reflectance spectrum) were used. This multiplier permitted an examination of the effects of modeled spectrum albedo on the number of spectra modeled within each constraint.

For the final comparison, models from all six land cover classes were combined and RMSE and spectral angle for the

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EAR-selected endmember models were compared using linear regression.

#### 4. Results

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Comparisons of RMSE and spectral angle for each land cover class demonstrated that the two error metrics are closely related (Fig. 2). Model error ranged widely within each spectral library. The chamise and grassland classes showed the most spectral variability within each class, with RMSE and spectral angle having high values on their respective axes. The ceanothus and impervious surface classes showed the least amount of spectral variability, with relatively low RMSE and spectral angles. Linear regression of spectral angle against RMSE revealed strong correlations between the two error metrics (Table 2).  $R^2$  values ranged from 0.87 for the impervious surface class to 0.99 for the



Fig. 4. Number of spectra (out of 50) modeled for each land cover class. The multiplier was used to reduce the albedo of the modeled spectra, and the five lines represent different RMSE constraints.

ceanothus class.  $R^2$  values for all six land cover classes were above 0.96, with the exception of the impervious surface class. Fitted slope and intercept values were also similar, and intercept values were near zero for all six land cover classes (Table 2).

Each of the scatterplots in Fig. 2 is roughly fan shaped, with low dispersion of points at lower RMSE and spectral angle and higher dispersion of points at high RMSE and spectral angle. A single spectrum modeled by the set of endmembers forms a line that indicates a fixed relationship between RMSE and spectral angle. Variations in the albedo of the modeled spectra create the fan shape. Since RMSE decreases as the non-shade endmember fraction decreases, the slope of the relationship between RMSE and spectral angle will decrease as the albedo of the modeled spectrum decreases. From this, it can be inferred that the range in albedo in the impervious surface and grass spectra is much larger than the range in albedo in the ceanothus, oak, and manzanita spectra (Fig. 2).

Since the albedo of the modeled spectrum determines the slope of the relationship between RMSE and spectral angle, the residuals of the linear regression between RMSE and spectral angle should be dependent on the length of the vector of the modeled spectrum. Fig. 3 compares the RMSE residuals for the six land cover classes calculated using the slope and intercept values from Table 2 to the length of the modeled spectrum vector. For each scatterplot there is a broad increase in the residual RMSE as the length of the modeled spectrum vector increases. In Fig. 3, an individual modeled spectrum modeled by many different endmembers forms a line of residuals parallel to the yaxis. The spread of the residuals is small where the slope of the trend for that particular modeled spectrum is close to the slope of the regression line. The spread of the residuals is much larger where the modeled spectrum is much darker or brighter than average, forming a "bow-tie" shape (Fig. 3).

The six endmembers selected by EAR were used to model their land cover classes using MESMA and SAM. To test whether the selected endmembers were favored by the MESMA model used by EAR, the equivalent minimum average spectral angle was also calculated. The minimum average spectral angle selected an identical set of endmembers when compared with those selected by EAR. The number of spectra modeled by the selected endmembers below a specific error constraint varied according to the constraint used (Tables 3 and 4). The MESMA standard error constraint of 2.5% reflectance (Roberts et al., 1998) modeled a similar number of spectra within each land cover class compared with a spectral angle constraint of 0.1 radians. MESMA included a slightly higher number of spectra than the standard error constraint for SAM. Both models demonstrated a steep reduction in the number of included modeled spectra for the most restrictive constraints.

Since RMSE is dependent on the albedo of the modeled spectrum, the number of spectra modeled within a specific

Fig. 5. Spectral angle vs. RMSE for all six land cover types. The EAR selected endmember for each land cover class was used to model that land cover class.

error constraint by MESMA should increase as the albedo of modeled spectra decrease. A multiplier was used to reduce the albedo of the modeled spectra, while the EAR selected endmembers were kept at constant albedo. The effects of varying the albedo of the modeled spectra can be seen in Fig. 4. The number of spectra modeled by each endmember increases as the albedo of the modeled spectra drops. For loose RMSE constraints, the number of additional spectra is relatively small (Fig. 4). As constraints tighten, however, the number of additional spectra included below the error constraint continually rises as the albedo of the modeled spectra is decreased.

Although differences in modeled spectrum albedo do produce variability in RMSE that is not present in spectral angle, the models run using the EAR selected spectra showed that the two metrics are nearly equivalent when carefully selected endmembers were used. Data points for spectral angle vs. RMSE for all six land cover classes are shown in Fig. 5. There is a strong apparent relationship between RMSE and spectral angle for the spectral classes examined. A linear regression of RMSE against spectral angle produces an  $R^2$  of 0.97. The correlation between the two error metrics is slightly lower if values above the 2.5% RMSE threshold are discarded, with an  $R^2$  of 0.94.

#### 5. Discussion

The correlations between RMSE and spectral angle demonstrate that the MESMA and SAM error metrics are not equivalent, but that they are closely related. For modeling spectra with low variability in albedo, MESMA



y = 21.085x + 0.0151

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Fig. 6. A schematic of error constraint selectivity. Endmember A and modeled spectrum B correspond to the vectors shown in Fig. 1. r is within the RMSE error constraint, and s is within the spectral angle error constraint. The darkest shaded area is the region where the two constraints overlap. Error constraints to the left of endmember A have been omitted for the purpose of clarity.

and SAM should produce equivalent results. The dependence of RMSE on the albedo of modeled spectra should be taken into account in images with high variability in the albedo of modeled spectra. Differences in solar illumination due to topography are of particular concern, since a partially shaded surface might fall below a given RMSE threshold, but a fully illuminated surface might not. Selection of spectral range and the number of bands may increase or decrease the albedo of the modeled spectra. Relationships between MESMA and SAM error metrics derived for full range spectra may not apply to convolved or subset spectra with different albedos.

The results also demonstrate the importance of error constraints when using either MESMA or SAM. Error constraints can be set loosely enough to include a large number of modeled spectra or tightly enough to include only those spectra that are most similar to the endmember. Given similar error constraints, using one model rather than another is unlikely to produce remarkably different results; differences will be much more pronounced when the error constraints themselves are varied. There is a difference in the selectivity of error constraints based on the albedo of the modeled spectrum (Fig. 6). Above a specific modeled spectrum albedo, marked by the dashed line in Fig. 6, a RMSE error constraint will include a smaller range of spectral variation than a similar spectral angle constraint. The opposite applies for modeled spectrum albedos below the dashed line. If similar error constraints are used for MESMA and SAM, MESMA will be more selective for modeled spectra with higher albedos while SAM will be more selective for modeled spectra with lower albedos (Fig. 6).

While MESMA provides fractional abundance of endmembers, it does have the drawback of the dependence of RMSE on the albedo of the modeled spectrum. Thankfully, the problem of spectral matching is not limited to an either/ or solution. MESMA could be adapted to use an error metric that is less sensitive to differences in modeled spectrum albedo. RMSE could be inversely weighted by the albedo of the modeled spectrum, so that lower albedo would produce higher RMSE values. Alternatively, error constraints could be weighted by albedo, allowing a tighter error constraint for lower albedo spectra and a looser error constraint for higher albedo spectra. A more promising approach might be a hybrid model that uses aspects of both models. Gillis and Bowles (2004) have proposed a hybrid model that uses endmembers derived from linear mixing to create a new coordinate system for SAM.

#### 6. Conclusions

Two commonly used spectral matching algorithms, MESMA and SAM, demonstrate similar results when applied to a spectral library containing five vegetation classes and an impervious surface class. Error metrics for MESMA and SAM are linearly related and highly correlated. Differences between these error metrics are due to differences in the albedos of modeled spectra.

In choosing between two competing spectral matching algorithms, each method has advantages and disadvantages. MESMA is the more flexible algorithm, providing the ability to calculate fractional abundance and incorporate additional endmembers where two endmembers are inadequate. Unlike MESMA, SAM is not sensitive to variations in the albedos of modeled spectra. Both models produce similar results for the two endmember case when used with properly selected endmembers. The selection of the error constraint appears to have a much greater impact on the number of spectral matches than the selection of matching algorithm. More effort should be invested in determining appropriate error constraints for both algorithms across a variety of spectral environments.

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