

Performance Analysis & Comparative Study of Geometrical Approaches for Spectral Unmixing

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Abstract— The hyperspectral cameras used for imaging is having low spatial resolution ,and thus the pixels in the captured image will be mixtures of spectra of various materials present in the scene.Then further analysis of images becomes a tough task.Thus spectral unmixing comes as an unavoidable step in hyperspectral image processing.Spectral unmixing aims at finding out the no. of reference substances(endmembers),their spectral signatures and corresponding abundance maps of them in a hyperspectral image.This paper presents a comparative study and performance analysis of 5 geometrical algorithms for spectral unmixing ,namely AVMAX,SVMAX,ADVMM,SDVMM and N-FINDR.All the 5 algorithms are applied to the real hyperspectral data set (cuprite data,Nevada,U.S) and results are validated with reference to U.S.G.S spectral library.

Index Terms— ADVMM, AVMAX, Hyperspectral imaging, N-FINDR, SDVMM, Spectral signature, Spectral unmixing , SVMAX,

1 INTRODUCTION

HYPERSPECTRAL sensors collect the data in hundreds of very narrow contiguous bands, and this provides a good way for the identification of various materials over the observed scene captured by the sensor. The various materials are discriminated on their unique spectral signatures. Hyperspectral imaging is having a wide range of applications in various fields as in agriculture, planetary remote sensing, military, environmental monitoring etc [1]. The hyperspectral imaging sensors can capture many contiguous bands which is having very high spectral resolution and this will be covering not only visible regions but also the infra red regions of electromagnetic spectrum (0.3-2.5 μ m) [2],[3]. Advanced hyperspectral sensors like AVIRIS [4] of NASA is now able to cover the above mentioned wavelength region using about 200 spectral channels.

In the case of hyperspectral images, depending upon the spatial resolution of sensor, the individual pixels in the captured scene may comprise of more than one material. Each pixel will be the mixture of various materials of the surface patch and thus the spectra observed will contain multiple endmembers (or spectral signatures) and thus the further analysis becomes difficult. This happens mainly because of the poor spatial resolution of the sensor used. Fig1 explains the concept of hyperspectral imagery [10]. There comes the need of hyperspectral unmixing. Hyperspectral unmixing aims at the decomposition of the observed spectra into a set of pure reference materials (endmembers) and their abundance fractions. Thus unmixing process gives both spectral signatures and corresponding abundance maps of materials present in the scene [5]. This unmixing problem has been a subject to

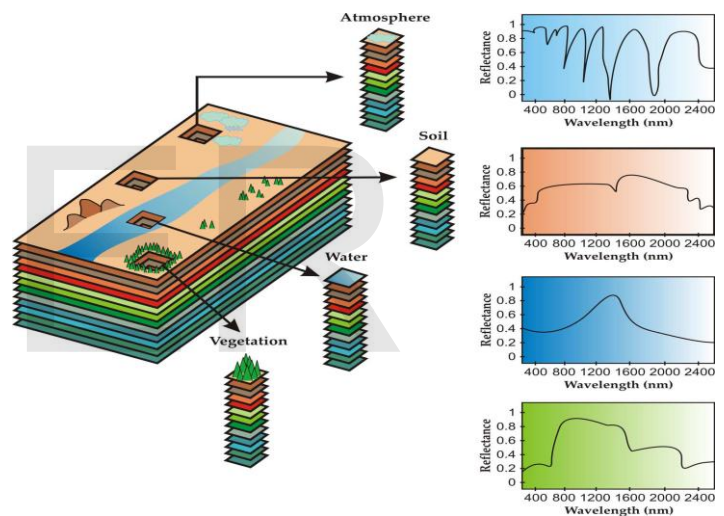


Fig1. Hyperspectral imagery.

1.1 Spectral unmixing

Hyper Spectral unmixing is basically a blind source separation problem [6],[35]. Hyperspectral sense contain sources which are statistically dependent and they may combine either in a linear or nonlinear fashion. This makes spectral unmixing problem to be placed in higher level compared to other source separation problems.

Unmixing can be classified to linear [7] and Non linear [8]. Linear models assume that the mixing scale is macroscopic, and the light which falls on the surface interacts with only one material. This type of mixing takes place due to the low spatial resolution of the sensor. Here multiple scatterings do not take place.

In the case of Nonlinear mixing models the interaction between the light which is scattered by multiple materials occurs, and the mixed model becomes complicated. The interactions can be at Intimate or microscopic level. Thus non-linear unmixing becomes a difficult task. So here this paper concentrates in linear unmixing due to its simplicity, and also it's the basis of many algorithms for more than 30 years.

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many investigative studies for the past many years.

1.2 Linear Spectral Unmixing

The linear mixing model assumes that the spectra of a pixel in the acquired scene is a linear combination of all pure materials (endmembers) present in the scene. It is assumed that the hyperspectral sensor used for capturing the scene has L spectral bands, linear mixing model can be mathematically represented as follows.

$$y = M\alpha + n \quad (1)$$

Where y is an $L \times 1$ column vector, M is an $L \times q$ matrix containing q endmembers (pure reference materials) and α is a $q \times 1$ vector containing the fractional abundances of the endmembers in the pixel and n is another $L \times 1$ vector indicating the errors which affect the measurements at each pixel [9]. In this modelling both M and α have to be found by unmixing. Here ANC (abundance non-negativity constraint) $\alpha_i \geq 0$, where $i=1,2,\dots,q$ and ASC (abundance sum to one constraint), $1^T \alpha = 1$

Are imposed to this model. This takes another fact into consideration as α_i , for $i=1,2,\dots,q$, represent the fractions or proportions of the pure materials or endmembers present in the scene. In this $Y \equiv \{y_i \in R^L, i=1,\dots,n\}$ of n no. of observed spectral vectors with dimension L .

Here in this paper all the 5 geometrical algorithms rely on this linear model in order to carry out the unmixing process. All the geometrical approaches try to solve the same linear unmixing problem shown in (1). Linear mixing concept is shown in fig. 2 [9]

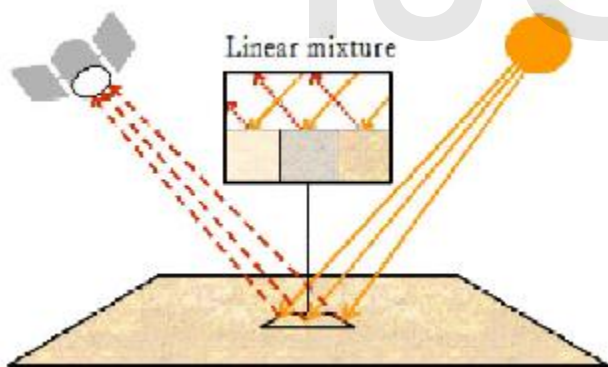


Fig2. Linear mixing model without any multiple scattering effects.

1.3 Endmember extraction algorithms-overview

Spectral unmixing algorithms can also be called as Endmember extraction algorithms, endmember identification algorithms etc. All the Spectral unmixing algorithms are mainly classified in to three types. They are statistical approaches, sparse based methods and geometrical approaches.

Statistical approaches are rarely used in the case of spectral unmixing, since their computational complexity level is very high when compared to other methods as sparse and geometrical methods. But still if the spectral mixtures are highly mixed then geometrical approaches provide poor results due to the lack of pure spectral vectors and all these statistical methods come to play. Under this, unmixing problem is formulated as a statistical inference problem and statistical methods like ICA (Independent component analysis) [11], DECA (dependent component analysis) [12] etc are the main algorithms coming under this category. All these are formulated under a Bayesian framework.

Sparse based approaches are the another category of spectral unmixing algorithms. In this spectral unmixing is formulated in a semi-supervised fashion, and it is assumed that the spectral signatures observed can be expressed as the linear combinations of known pure spectral signatures from a spectral library [13], [14]. OMP (orthogonal matching pursuit) [15], ISMA (iterative spectral mixture analysis) [16] etc comes under this. The most popular algorithms coming under this category are SUNSAL (sparse unmixing via splitted and augmented lagrangian approach) [17], and SUNSAL-TV (sparse unmixing via splitted and augmented lagrangian-total variation) [18].

Geometrical approaches come as the third category of spectral unmixing algorithms. Basically it follows the fact that, under the linear mixing model spectral vectors belong to the simplex set whose vertices correspond to the endmembers. Thus by finding out the vertices it is possible to find out the endmember in the hyperspectral image. There are two categories in this approach. Algorithms which assume the presence of pure pixels come under the one category and algorithms which do not assume the presence of pure pixels come under another category. MVSA (minimum volume simplex analysis) [19], MVES (minimum volume enclosing simplex) [20], SISAL (simplex identification via split and augmented lagrangian) [21], etc comes under the first category. In the second category to which this paper concentrates, come the following algorithms like SVMAX (successive volume maximization) [22], AVMAX (Alternating volume maximization) [22], ADVMM (alternating decoupled volume maximization) [23], SDVMM (successive decoupled volume maximization) [23], N-FINDR [24], VCA (vertex component analysis) [25], IEA (iterative error analysis) [26], PPI (pixel purity index) [27], etc are some of the algorithms come under this section. In this paper 5 popular algorithms of this category namely AVMAX, SVMAX, ADVMM, SDVMM and N-FINDR is taken in to account and their performance is evaluated and results are compared to find out the good one giving the best result among them.

The rest of the paper is organized as follows. Section 2 gives the theoretical ideas behind the selected algorithms, Section 3 explains the metrics used for performance evaluation, Section 4 presents the experiments with real hyperspectral data its results and the performance analysis and finally conclusions are drawn in Section 5.

2 PURE PIXEL BASED GEOMETRICAL ALGORITHMS

As discussed in the previous sections geometrical algorithms with pure pixel assumption assumes the presence of atleast one pure pixel per endmember. These pure pixel algorithms still belong to minimum volume class. This assumption of pure pixels make these algorithms very efficient but still creates difficulty in some datasets. In this section a brief theoretical side of each of the 5 algorithms namely AVMAX, SVMAX, ADVMM, SDVMM and N-FINDR is given.

2.1 AVMAX (Alternating volume maximization)

Alternating volume maximization algorithm [22] is based on winter problem described in [28]. In winter's work he proposed that the ground-truth endmembers can be located by finding a collection of pixel vectors whose simplex volume is the largest. The optimization formulation of winter's problem is as follows.

$$\begin{aligned} \max_{v_1, \dots, v_N \in R^{N-1}} \quad & vol(v_1, \dots, v_N) \\ \text{s.t} \quad & v_i \in conv\{x[1], \dots, x[L]\}, \quad i = 1, \dots, N \end{aligned} \quad (2)$$

Where according to winter's work each endmember estimate v_i is restricted to be any vector in $\{x[1], \dots, x[L]\}$. When alternating volume maximization is applied to this it maximizes in a cyclic fashion, the volume of the simplex defined by the pure members (endmembers) but with respect to only one endmember at a time. This is explained as follows in [22].

The starting point is taken as (v_1, \dots, v_N) . The following alternating cycle is repeated as for $j=1 \dots N$ solve the problem

$$\max_{v_j \in F} \det(\Delta(v_1, \dots, v_{j-1}, v_j, v_{j+1}, \dots, v_N)) \quad (3)$$

And update v_j as the solution of (3). We have to continue this until the stopping criterion is satisfied. The algorithm is explained in detail in [22]. Avmax is somewhat similar to SC-N-FINDR which is a modified version of N-FINDR described in [29].

2.2 SVMAX (Successive volume maximization)

Successive volume maximization [22] is another strategy of optimization for the winter's problem shown in (2). This requires the winter's problem to be written in a modified fashion as follows in [22].

$$\begin{aligned} \max_{w_1, \dots, w_N \in R^N} \quad & |\det(w)| \\ \text{s.t} \quad & w_i \in \bar{F}, \quad i = 1, \dots, N \end{aligned} \quad (4)$$

Where $\bar{F} = \{w \in R^N \mid w = [v^T \ 1]^T, v \in F\}$

Then according to rules $|\det(w)|$ can be written as follows.

$$|\det(w)| = \sqrt{|\det(w^T w)|} \quad (5)$$

Thus (4) is modified as follows

$$\begin{aligned} \max_{w_1, \dots, w_N \in R^N} \quad & f_1(w_1) f_2(w_1, w_2) \dots f_N(w_1, \dots, w_N) \quad (6) \\ \text{s.t} \quad & w_i \in \bar{F}, \quad i = 1, \dots, N. \end{aligned}$$

Where $f_1(w_1) = \|w_1\|_2$
 $f_j(w_1, \dots, w_j) = \|P \perp_{w_{1:(j-1)} w_j}\|_2, \quad j = 2, \dots, N$

Thus the following procedure is followed.
 For $j=1:N$ solve the problem

$$W_j = \arg \max_{w_j \in \bar{F}} f_j(w_1, \dots, w_{j-1}, w_j) \quad (7)$$

At last we will get (w_1, \dots, w_N) as the approximate solution of (6). It's similar to VCA [25] in some aspects. But unlike VCA algorithm SVMAX considers the whole subspace when the data is projected orthogonally whereas VCA takes random direction in subspace.

2.3 ADVMM (Alternating decoupled volume max-min)

In this winter's problem shown in (2) is formulated as a max-min problem and alternating optimization [23] is used to solve it. This winter's worst case problem is given as a max-min problem as follows in [30].

$$\begin{aligned} \max_{\substack{v_i \in R^{N-1} \\ i=1, \dots, N}} \quad & \left\{ \min_{\substack{\|u_i\| \leq r \\ i=1, \dots, N}} |\det(\Delta(v_1 - u_1, \dots, v_N - u_N))| \right\} \quad (8) \\ \text{s.t} \quad & v_i \in conv\{y[1], \dots, y[L]\}, \quad i = 1, \dots, N \end{aligned}$$

Where $y[1] \dots y[L]$ is the data cloud inside which maximum volume simplex is situated. From the vertices of this simplex endmembers are to be found out.

By taking $v_i = Y\theta_i$, $Y = [y[1], \dots, y[L]] \in R^{(N-1) \times L}$ and for any permutation matrix p , $\det(P\Delta) = \pm \det(\Delta)$ we can write the problem in (8) as

$$\max_{\substack{\theta_i \in S \\ i=1, \dots, N}} \left\{ \min_{\substack{\|u_i\| \leq r \\ i=1, \dots, N}} \det(\Delta(Y\theta_1 - u_1, \dots, Y\theta_N - u_N)) \right\} \quad (9)$$

Then by doing the cofactor expansion and simplification of (9) as in [30] it is reduced to

$$\max_{\theta_j \in S} \left\{ \min_{\|u_j\| \leq r} k_j^T (\Delta(Y\theta_j - u_j)) \right\} \quad (10)$$

The above problem can be solved by solving the 2 decoupled problems shown below.

$$u_j = \arg \max_{\|u_j\| \leq r} k_j^T u_j = rk_j / \|k_j\| \quad (11)$$

$$\theta_j = \arg \max_{\theta_j \in S} k_j^T Y\theta_j = e_l, \quad l = \arg \max_{n=1, \dots, L} k_j^T y[n] \quad (12)$$

Thus ADVMM solves the max-min problem of spectral unmixing.

2.4 SDVMM(Successive decoupled volume max-min)

This is also another algorithm which follows winter’s problem shown in (8).This solves the decoupled max-min problem in a successive optimization method. By assuming

$$w_i = [v_i^T \ 1]^T, z_i = [u_i^T \ 0]^T \ \& \ y[n] = [y[n]^T \ 1]^T$$

Problem(8) can be written as follows.

$$\max_{w_i \in F, i=1, \dots, N} \{ \min_{\substack{\|z_i\| \leq r \\ e_N^T z_i = 0, \forall i}} | \det([w_1 - z_1, \dots, w_N - z_N]) | \} \quad (13)$$

Where $F = \text{conv}\{y[1], \dots, y[L]\}$. The problem (13) can be modified and written as

$$\max_{w_i \in F, i=1, \dots, N} \min_{\substack{\|z_i\| \leq r \\ e_N^T z_i = 0, \forall i}} \prod_{j=1}^N f((w_1, z_1), \dots, (w_j, z_j)) \quad (14)$$

where

$$f((w_1, z_1), \dots, (w_j, z_j)) = \left\| P_{H_{1:(j-1)}}^\perp (w_j - z_j) \right\|, \quad (15)$$

The detailed explanation of terms and simplification steps is given in [30].The problem can be approximated by successive optimization as follows.

$$(w_j, z_j) = \arg \max_{w_i \in F, i=1, \dots, N} \min_{\substack{\|z_i\| \leq r \\ e_N^T z_i = 0, \forall i}} f((w_1, \hat{z}_1), \dots, (w_j, \hat{z}_j)) \quad (16)$$

The solution to (16) is given in [30] as follows.

$$\hat{z}_j = \arg \min_{\|z_j\|_2 \leq r} \left\| P_{H_{1:(j-1)}}^\perp (w_j - z_j) \right\| \quad (17)$$

$$w_j = \bar{y}[l], l = \arg \max_{H_{1:(j-1)}} \left\| P_{H_{1:(j-1)}}^\perp w_j \right\| \quad (18)$$

Thus it solves the max-min problem by successive optimization.

2.5 N-FINDR

This is another popular algorithm used for spectral unmixing.This also works according to winter’s belief [24].This is a pure pixel based algorithm and this search for the set of pixels with largest possible volume by inflating a simplex inside the given dataset.

The original n-findr algorithm [31] is having 4 steps as follows.

1) Feature reduction-In this the dimension of data is reduced from n to P-1 by some PCA [32] or MNF[33],where P is the number of endmembers to be identified.

2)Take some randomly selected endmembers from the dataset as $\{E_1^{(0)}, E_2^{(0)}, E_3^{(0)} \dots E_p^{(0)}\}$

3)At each iteration $k \geq 0$, calculate the volume by this set of endmembers as follows.

$$v(E_1^{(k)}, E_2^{(k)}, \dots, E_p^{(k)}) = \frac{|\det \begin{bmatrix} 1 & 1 & \dots & 1 \\ E_1^{(k)} & E_2^{(k)} & \dots & E_p^{(k)} \end{bmatrix}|}{(p-1)!} \quad (19)$$

4) Replacement- For each and every pixel the volume corresponding to it is checked by this way,if this pixel replaces one of the given endmember positions in matrix shown above.. If the replacement of pixel results in an increase in volume,the pixel replaces the endmember.This process continues until there are no endmember replacements in the given data.

3 METRIC USED FOR PERFORMANCE EVALUATION

As the result of spectral unmixing we will get spectral signatures of endmembers and also their corresponding abundance maps. Here in this paper The metric used for the validation of results is Spectral Angle Mapper (SAM)[34]. It’s measured between the original library spectra which we will get from U.S.G.S library [36], and the spectra obtained by the unmixing process.

The basic equation for the spectral angle is given as follows.

$$\theta(x, y) = \arccos \frac{\langle x, y \rangle}{\|x\| \|y\|} \quad (20)$$

Where, x is the library spectra and y is the spectra obtained from unmixing.As the spectral angle (SA) decreases, the result becomes more good and when we get a high value for SA we can infer that the performance of algorithm is poor.In that way we calculate the SA for each mineral spectra and finally average the results to obtain average SA for each algorithms.This can be seen in detail in the following sections

4 EXPERIMENTS ON REAL DATA-RESULTS AND PERFORMANCE ANALYSIS

In this part,all the 5 mentioned algorithms AVMAX,SVMAX,ADVMM,SDVMM and N-FINDR are applied to the real hyperspectral data set taken over Cuprite mining site,Nevada,in 1997[37].We consider only a subimage of the hyperspectral data as a region of interest ,which is of size 250x191 pixels(L=47750).This contains 224 bands over the wavelength region of 0.4µm to 2.5 µm.In this set, the bands 1-2,104-113,148-167 and 221-224 were removed due to low SNR

effect which occurs due to the effect of water vapour. Thus a total of 188 bands were used for the implementation of the algorithms. As the next step, we want to know how many endmembers are located in this region of interest. For this we applied Hyperspectral subspace identification by minimum error (HySime) [38] and thus estimated the number of endmembers in this region as $N=18$.

The abundance maps corresponding to each mineral was obtained by using fully constrained least square (FCLS) [39] method. The minerals obtained were then identified by the visual comparison of the abundance maps obtained with the abundance maps shown in [20],[25],[40], and [41]. As said earlier spectral angle is used for as measure for the performance. The value of SA for the estimated endmembers obtained by all the 5 algorithms are shown in Table 1,2,3,4 and 5. The numbers in parentheses denote the value of SA for the estimated endmember which is repeated. Due to the space limit here we have shown the estimated endmember signatures and abundance maps of N-FINDR algorithm and repeated minerals are not shown. The abundance maps and spectral signatures are shown below.

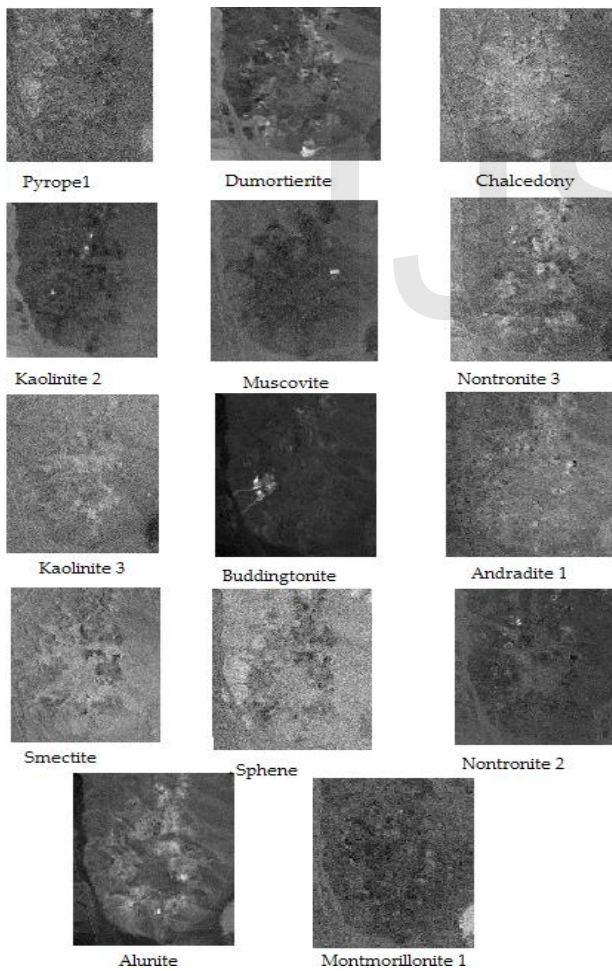


Fig.3. Abundance maps obtained by N-Findr algorithm

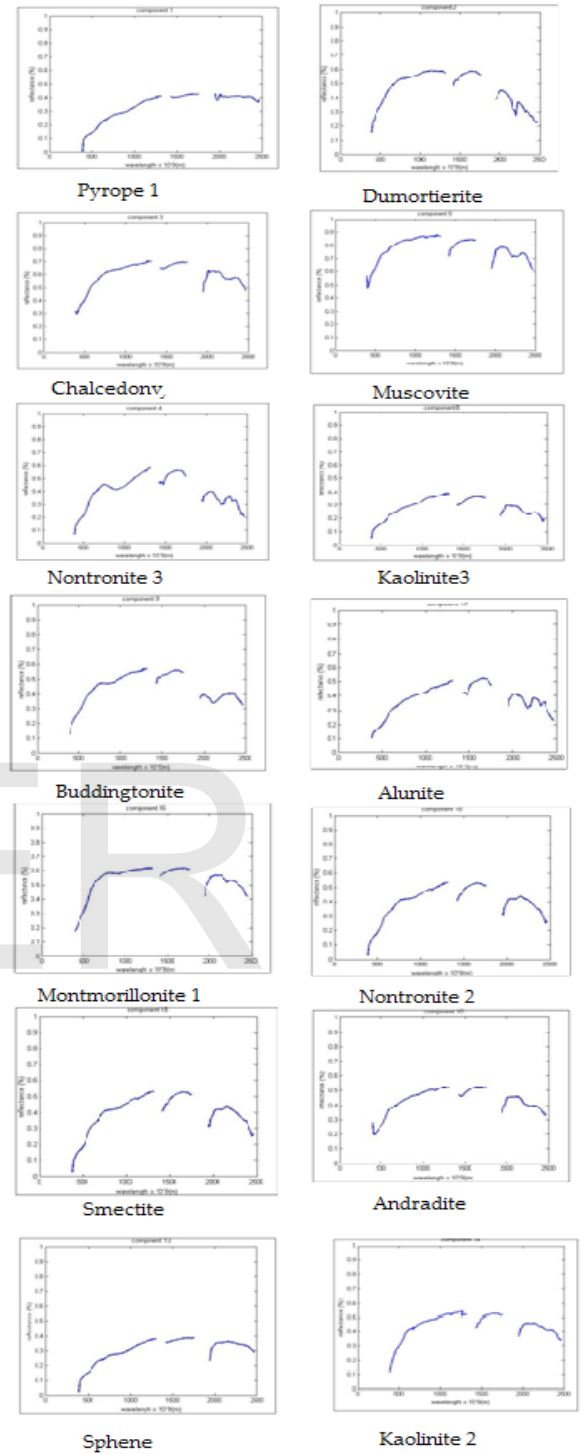


Fig.4. Spectral signatures estimated by N-findr algorithm

TABLE 1
SA values for AVMAX algorithm

Minerals	SA(In degrees)
1) Buddingtonite	4.3752
2) Nontronite2	4.0603
3) Nontronite3	8.5687(13.9465)
4) Muscovite	7.5151(8.1180)
5) Dumortierite	9.9103(6.1794)
6) Montmorillonite 1	7.5419(8.4586)
7) Alunite	14.2029(11.6362)
8) Nontronite1	23.8962
9) Andradite1	6.9561
10) Kaolinite1	8.4594
11) Chalcedony	5.8523
12) Smectite	4.7384
13) Desert varnish	11.9521
Average SA	9.2418

TABLE2
SA values for SVMAX algorithm

Minerals	SA (In degrees)
1) Muscovite	7.9462
2) Alunite	4.5523(12.5400)
3) Kaolinite 1	20.6245(8.4594)
4) Dumortierite	9.9103(6.5689)
5) Montmorillonite 1	7.3248
6) Buddingtonite	3.9375
7) Nontronite 3	8.9030(6.7681)
8) Smectite	5.9870
9) Nontronite2	3.6690(4.9857)
10) Paragonite	6.3562
11) Desertvarnish	6.3356
12) Chalcedony	4.8207
13) Goethite	14.4817
Average SA	8.0094

TABLE 3
SA values for ADVMM algorithm

Minerals	SAD (In degrees)
1) Paragonite	6.3317(6.5816)
2) Nontronite2	3.6689(4.9378)
3) Muscovite	8.1111
4) Buddingtonite	4.3754
5) Goethite	20.9323
6) Andradite1	8.2735
7) Alunite	7.4632(8.3189)
8) Smectite	3.2023
9) Montmorillonite 1	7.2620
10) Kaolinite1	11.9986(21.2243)
11) Dumortierite	6.2242(6.8216)
12) Chalcedony	8.9438
13) Desert varnish	6.1276
Average SA	8.3777

TABLE 4
SA values for SDVMM algorithm

Minerals	SA (In degrees)
1) Muscovite	7.9462
2) Nontronite 3	15.0209(8.9030)
3) Kaolinite 1	20.6244
4) Dumortierite	5.0531(9.9100)
5) Montmorillonite 1	7.3245
6) Buddingtonite	3.9378
7) Nontronite2	3.6689(4.9857)
8) Smectite	3.5697(5.9868)
9) Alunite	12.5399(8.0169)
10) Desertvarnish	6.3356
11) Paragonite	6.0918
12) Chalcedony	4.8207
13) Goethite	14.4815
Average SA	8.2898

TABLE 5
SA values for N-FINDR algorithm

Minerals	SA (In degrees)
1)Pyrope 1	3.6341
2)Dumortierite	5.0531(11.9325)(9.9103)
3)Chalcedony	5.222
4)Kaolinite 2	10.8546
5)Muscovite	7.6819
6)Nontronite 3	7.9865
7)Kaolinite 3	10.4473
8)Buddingtonite	4.3752
9)Andradite	8.9945
10)Smectite	4.7384
11)Nontronite2	6.5617(3.9298)
12)Sphene	6.8655
13)Alunite	5.3319(15.3751)
14)Montmorillonite 1	7.5419
Average SA	7.5745

The tables shown above gives the Spectral angle between the estimated endmember signatures and the Library spectra of U.S.G.S library. When analyzing the tables we can see that the Average Spectral angle is different for all the five algorithms and AVMAX(Alternating Volume maximization)algorithm gives the high value for the average SA which is 9.24. This gives the indication of poor performance when compared to other algorithm. In between the algorithms N-FINDR gives the appreciable result with Average SA of 7.4131. This points towards a good result of spectral unmixing of the given data set. All the other algorithms could identify only 13 minerals out of 18 whereas N-FINDR could identify 14 minerals out of 18. (In the table it can be seen that Alunite and Nontronite 2 were repeated, and Dumortierite was repeated 3 times). Moreover N-FINDR was able to detect the rare mineral "sphene" where other 4 algorithms was not able to detect the presence of it. In between N-findr and Avmax, comes the rest of algorithms and in this Svmax gives the good performance after N-findr, Sdvmm comes as the third and Advmm comes as the second last when looking in to the performance level.

As the N-findr algorithm works on the replacement of pixels and endmembers it does not miss any endmembers in the given data set and can give the better result when compared to all other algorithms. It solves the winter's problem in an efficient way compared to all other algorithms and comes out with the best result among the other methods.

5 CONCLUSION

In this paper, the implementation and comparative study of five geometrical approaches which are popularly used for spectral unmixing is done. The spectral unmixing experiment

was done with Cuprite dataset(Nevada,U.S).The performance comparison of algorithms is done based on Spectral Angle mapper and it used U.S.G.S library as the reference. By the comparative study it's found that N-FINDR algorithm gives the better performance compared to the other four algorithms. AVMAX (Alternating volume maximization) is the one which gives much lower performance compared to others. As a future work the geometrical based spectral unmixing techniques can be compared with the statistical methods and sparse methods and it can make out new results. This can open new ways to researches also.

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