Endmember Extraction from Hyperspectral Image Based on Discrete Firefly Algorithm (EE-DFA)

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Abstract

This study proposed a novel method to extract endmembers from hyperspectral image based on discrete firefly algorithm (EE-DFA). Endmembers are the input of many spectral unmixing algorithms. Hence, in this paper, endmember extraction from hyperspectral image is regarded as a combinational optimization problem to get best spectral unmixing results, which can be solved by the discrete firefly algorithm. Two series of experiments were conducted on the synthetic hyperspectral datasets with different SNR and the AVIRIS Cuprite dataset, respectively. The experimental results were compared with the endmembers extracted by four popular methods: the sequential maximum angle convex cone (SMACC), N-FINDR, Vertex Component Analysis (VCA), and Minimum Volume Constrained Nonnegative Matrix Factorization (MVC-NMF). What's more, the effect of the parameters in the proposed method was tested on both synthetic hyperspectral datasets and AVIRIS Cuprite dataset, and the recommended parameters setting was proposed. The results in this study demonstrated that the proposed EE-DFA method showed better performance than the existing popular methods. Moreover, EE-DFA is robust under different SNR conditions.

Key words

Endmember Extraction, Discrete Firefly Algorithm (DFA), Hyperspectral Image, Remote Sensing

27 1 Introduction

28 Hyperspectral remote sensing acquires image covering hundreds of narrow contiguous spectral
29 bands, which provides a contiguous spectrum for each pixel [1]. However, due to the relative low spatial
30 resolution of hyperspectral image, it is inevitable that several materials are presented together in one
31 pixel in natural environment. Thus, it has triggered a popular research interest to determine the
32 abundance fraction of each material in a mixed pixel from hyperspectral image, which called spectral
33 unmixing. The first step for solving this problem (spectral unmixing) is usually endmember extraction
34 (EE), which is to determine the idealized pure spectral signature of each material. In fact, an endmember
35 extracted from a real hyperspectral image is generally still a mixed pixel that contains high fraction of
36 one kind of material [2]. In computer science and mathematics, discrete optimization is a topic on finding
37 a best object from a finite set of objects. In detail, discrete optimization problem is to find a combination
38 of discrete variables from all feasible solutions to optimize the objective function. What's more,
39 endmember extraction from a hyperspectral image is to find some pixels and combine them as pure
40 spectral signatures of the materials in the image to get the best accuracy of spectral unmixing results. In
41 this sense, endmember extraction from hyperspectral image can be transferred into a typical discrete
42 optimization problem that is of particular importance for spectral unmixing of hyperspectral image.

43 For recent more than two decades, many methods for endmember extraction from hyperspectral
44 image have been proposed. Typical algorithms developed for endmember extraction include pixel purity
45 index (PPI) [3], [4], N-FINDR [5], iterative error analysis (IEA) [6], vertex component analysis (VCA)
46 [7], the sequential maximum angle convex cone (SMACC) [8], the optical real-time adaptive spectral
47 identification system (ORASIS) [9], convex cone analysis (CCA) [10], automated morphological
48 endmember extraction (AMEE) [11], iterated constrained endmembers (ICE) [12], the single individual
49 evolutionary (SIE) strategy [13]. In addition, some new methods for endmember extraction were also
50 proposed in recent years [14-23]. In fact, currently, although there are a variety of methods for
51 endmember extraction from hyperspectral image, these methods have respective shortcomings.
52 Comparative analysis and discussions on the existing endmember extraction algorithms have been
53 conducted by several scholars [2], [19], [24]. In this paper, disadvantages of several typical algorithms
54 are displayed as examples. For instance, the PPI algorithm is a typical manual/interactive endmember

55 extraction method, which is slow and artificially influenced [2]. In the N-FINDR algorithm, it is
56 generally inevitable to reduce the dimensions of the hyperspectral dataset [5]. What's more, many
57 algorithms including the N-FINDR algorithm, VCA algorithm, SMACC algorithm etc., are based on a
58 simple geometrical precondition that the endmembers are the vertexes of a convex simplex in spectral
59 space [5], [7], [8]. However, due to some non-linear factors and the noise in a real hyperspectral image,
60 this precondition is not reliable [7]. Thus, the existing algorithms are still limited and it is necessary to
61 propose new algorithms with particular advantages to conduct endmember extraction from hyperspectral
62 image and provide more optional methods for endmember extraction for scholars in the area of
63 hyperspectral remote sensing.

64 Firefly algorithm (FA) is a novel nature-inspired algorithm, which is inspired by social behavior of
65 fireflies and was presented by Xin-She Yang [25]. It has been proven that FA is an efficient method to
66 solve optimization problem and is better than both particle swarm optimization (PSO) algorithm and
67 genetic algorithm (GA) in the respects of both efficiency and success rate [26], [27]. Moreover, Ref. [27]
68 has demonstrated that discrete firefly algorithm (DFA) performed better than the ant colony optimization
69 (ACO) algorithm in solving discrete optimization problems. Hence, DFA provides a better way for
70 solving discrete optimization problems including endmember extraction from hyperspectral image, than
71 other popular swarm intelligence algorithms, such as PSO, GA and ACO.

72 This paper proposes an endmember extraction method from hyperspectral image based on discrete
73 firefly algorithm (EE-DFA). To the best of our knowledge, there is little information available in
74 published literature about the application of firefly algorithm on endmember extraction. To realize the
75 endmember extraction, we redefined the objective function and several variables in FA, and proposed a
76 new discretization method of the firefly algorithm.

77 **2 Firefly Algorithm (FA)**

78 A brief introduction to FA is presented here, with the purpose to define necessary concepts to
79 explain the EE-DFA. More details of FA can be found in the Ref. [28]. Nature-inspired algorithms are
80 among the most important and powerful methods for optimization problems. In the nature, most firefly
81 species produce short and rhythmic flashes that is to act as a signal system to attract other fireflies.
82 Therefore, FA obeys the following rules: (1) All fireflies are attractive to other fireflies regardless of their

sex; (2) the attractiveness of a firefly is determined by its brightness, which means that for any two flashing fireflies the less bright one will move towards the brighter one. If a particular firefly is the brightest in the firefly population, it will move randomly; and (3) the brightness of a firefly is determined by the objective function. For a minimization problem in this study, the brightness of a firefly should be inversely proportional to the value of the objective function [27].

Distance: In FA, the distance r_{ij} of two fireflies $\mathbf{x}_i$ and $\mathbf{x}_j$ can be determined as follows.

$$r_{ij} = \sqrt{\sum_{k=1}^n (x_{ik} - x_{jk})^2} \quad (1)$$

where x_{ik} is the k -th component of the i -th firefly $\mathbf{x}_i$ and n is the number of components of the firefly $\mathbf{x}_i$. Here we give an explanation on the word ‘component’. ‘component’ is used to express a dimension of a vector. For example, if there is a vector $\mathbf{V} = (a, b, c, d, e, f)$, we could say that the vector $\mathbf{V}$ possesses 6 components and “ d ” is the 4th component of the vector $\mathbf{V}$.

Attractiveness: The attractiveness β_{ij} between two fireflies $\mathbf{x}_i$ and $\mathbf{x}_j$ is a monotonically decreasing function. For instance, it can be the following form.

$$\beta_{ij} = \beta_0 e^{-\gamma r_{ij}^2} \quad (2)$$

where r_{ij} is the distance between two fireflies $\mathbf{x}_i$ and $\mathbf{x}_j$, β_0 is the attractiveness at $r_{ij} = 0$ and γ is a fixed light absorption coefficient.

Movement: The movement of the i -th firefly $\mathbf{x}_i$, when it is attracted by another brighter one ($\mathbf{x}_j$), can be determined as follows.

$$x_{ik} = x_{ik} + \beta_0 e^{-\gamma r_{ij}^2} (x_{jk} - x_{ik}) + \alpha(\text{rand} - 0.5) \quad (3)$$

where the second term is for the attraction between two fireflies, and the third term is randomization with α being the randomization step and “rand” is a random number uniformly distributed in [0, 1]. Equation (3) takes x_{ik} as an example to illustrate the calculation method of the components of $\mathbf{x}_i$ after one movement. All the components of $\mathbf{x}_i$ should be calculated according to equation (3) in one movement of $\mathbf{x}_i$.

To apply the FA on endmember extraction, we redefined the inputs, outputs, objective function, the meaning of fireflies, and proposed discretization method.

106 3 Endmember Extraction Based on Discrete Firefly Algorithm (EE-DFA)

107 3.1 Definition of the parameters and variables

108 In this section, the meaning of all the parameters and variables in EE-DFA is presented.

109 m : Number of endmembers that will be extracted.

110 n : Number of candidate endmembers and also the number of components of the firefly $\mathbf{x}_i$.

111 N : Number of the pixels in one spectral band.

112 L : Number of spectral bands in hyperspectral dataset.

113 t : $t=0$ means the i -th firefly is the current best solution in all fireflies. Otherwise, the i -th firefly is not the
114 current best solution in all fireflies.

115 $\mathbf{p}_i = (p_{i1}, p_{i2}, p_{i3}, \dots, p_{iL}), i=1, 2, 3, \dots, N$: The spectral reflectance of the i -th pixel.

116 $\mathbf{p}'_i = (p'_{i1}, p'_{i2}, p'_{i3}, \dots, p'_{iL}), i=1, 2, 3, \dots, N$: The approximate estimation of $\mathbf{p}_i$.

117 $\mathbf{e}_j = (e_{j1}, e_{j2}, e_{j3}, \dots, e_{jL}), j=1, 2, 3, \dots, m$: The spectral reflectance of the j -th endmember.

118 $a_{ij}, i=1, 2, 3, \dots, N, j=1, 2, 3, \dots, m$: The abundance fraction of the j -th endmember in the i -th pixel.

119 $a'_{ij}, i=1, 2, 3, \dots, N, j=1, 2, 3, \dots, m$: The least square estimation of a_{ij} .

120 $\mathbf{x}_i = (x_{i1}, x_{i2}, x_{i3}, \dots, x_{ik}, \dots, x_{in}), x_{i1}+x_{i2}+x_{i3}+\dots+x_{in}=m, x_{ik} \in \{0, 1\}$: The i -th firefly, also a feasible solution.

121 $x_{ik}=1$ means that the k -th candidate endmember is selected, otherwise is not.

122 $I(i)$: The brightness of the i -th firefly $\mathbf{x}_i$.

123 x_{best} : The firefly that is the best solution.

124 I_{best} : The brightness of the firefly that is the best solution.

125 $\mathbf{Y} = \{(y_1, y_2, y_3, y_4, \dots, y_n) \mid y_1+y_2+y_3, \dots, +y_n=m, y_i \in \{0, 1\}\}$: A feasible solution space including all the
126 feasible solutions.

127 3.2 Determination of the objective function

128 In the linear spectral mixture analysis (LSMA), the abundance fraction of the j -th endmember in the
129 i -th pixel (a_{ij}) obeys to the following equations (4) - (6) [29].

$$\mathbf{p}_i \approx \sum_{j=1}^m a_{ij} \mathbf{e}_j + \mathbf{r}_i \quad (4)$$

$$\sum_{j=1}^m a_{ij} = 1, \forall i \quad (5)$$

$$a_{ij} \geq 0, \forall i, \forall j \quad (6)$$

130 The full constraints least square (FCLS) is a method to obtain the abundance fraction a_{ij} , which
 131 obeys to all the equations (4) - (6) [29]. When all the endmembers ($\mathbf{e}_j, j=1, 2, 3, \dots, m$) are determined,
 132 based on the FCLS, a_{ij}' (the least square estimation of a_{ij}) can be acquired, which is the process of spectral
 133 unmixing. $\mathbf{p}_i'$ (the estimation of $\mathbf{p}_i$) can be obtained according to the following equation.

$$\mathbf{p}_i' = \sum_{j=1}^m a_{ij}' \mathbf{e}_j \quad (7)$$

134 As already mentioned in the introduction section, endmember extraction from a hyperspectral
 135 image is to find some pixels as pure spectral signatures of materials to get the best spectral unmixing
 136 results. The spectral unmixing results can be evaluated by the root-mean-square error (RMSE) between
 137 the real reflectance $\mathbf{p}_i$ and its estimation $\mathbf{p}_i'$, which can be calculated according to the following equation.

$$RMSE = \frac{1}{N} \sum_{i=1}^N \sqrt{\frac{1}{L} \sum_{j=1}^L (p'_{ij} - p_{ij})^2} \quad (8)$$

138 A less RMSE means a better result of spectral unmixing and also endmember extraction. Thus, the
 139 brightness $I(\mathbf{x})$ of the firefly $\mathbf{x}$ was defined as the opposite value of the RMSE.

$$I(\mathbf{x}) = -RMSE \quad (9)$$

140 Hence the problem of endmember extraction from hyperspectral image is to find the firefly $\mathbf{x}$ that
 141 corresponds to the maximum brightness $I(\mathbf{x})$, which could be formulated in a mathematical way as
 142 follows:

$$\begin{aligned} &\text{maximize } I(\mathbf{x}) \\ &\text{subject to } \mathbf{x} \in \mathbf{Y} \end{aligned} \quad (10)$$

143 3.3 Discretization of FA

144 The i -th firefly $\mathbf{x}_i$ ($\mathbf{x}_i = (x_{i1}, x_{i2}, x_{i3}, \dots, x_{ik}, \dots, x_{in}), x_{i1}+x_{i2}+x_{i3}+\dots+x_{in}=m, x_{ik} \in \{0, 1\}$) represents a
 145 feasible solution for endmember extraction. $x_{ik}=1$ means that the k -th candidate endmember is selected,
 146 otherwise is not. When the i -th firefly moves toward the j -th firefly, the position of the i -th firefly is
 147 recalculated based on (3) and thus changed from a binary number to a real number. To translate this real
 148 number to a binary number, this paper proposes a discretization method: the first m largest components
 149 of $\mathbf{x}_i$ is defined as 1 and other components is defined as 0. Here we give an example to illustrate this

150 discretization method, when $m=7$.

151 Before discretization: $\mathbf{x}_i = (1.0294, 1.0116, 0.2540, 1.1268, 1.2647, 0.1951, 0.2570, 1.0938, 1.1150,$
 152 $1.0298, 0.3152, 1.0412, 1.1143, 0.9708, 1.1006, 0.2838, 0.8435, 1.0315, 1.0844)$. The first seven
 153 (Because m equals 7) largest components of $\mathbf{x}_i$ is 1.1268, 1.2647, 1.0938, 1.1150, 1.1143, 1.1006 and
 154 1.0844.

155 Hence, after discretization: $\mathbf{x}_i = (0, 0, 0, 1, 1, 0, 0, 1, 1, 0, 0, 0, 1, 0, 1, 0, 0, 0, 1)$. This example is just
 156 used to explain the proposed discretization method and has nothing to do with the experimental data in
 157 this paper.

158 3.4 Process of the proposed EE-DFA method

159

160 Fig. 1 The flow chart of the procedure of the proposed EE-DFA

161 The main steps of the proposed EE-DFA method is presented in Fig. 1. The key processes are
 162 described as follows.

163 (1). The parameters and variables that need to be initialized include β_0 , γ , α , FireflyNumber (the number
 164 of fireflies, see the Section 4.2), Fireflies and their brightness. The analysis on the initialization of β_0 , γ ,
 165 and α could be found in the Section 4.3. According to the definition of fireflies, for the initialization of
 166 the firefly $\mathbf{x}_i$, we randomly set m components as 1 and other components as 0. The brightness $\mathbf{I}(\mathbf{x}_i)$ could
 167 be calculated based on FCLS and Equation (7) ~ (9).

168 (2). The implementation method of this step is shown as follows.

169 for $i = 1$: FireflyNumber

170 for $j = 1$: FireflyNumber

171 if ($\mathbf{I}(\mathbf{x}_j) > \mathbf{I}(\mathbf{x}_i)$)

172 Move $\mathbf{x}_i$ to $\mathbf{x}_j$ and update $I(\mathbf{x}_i)$

173 end if

174 end for j

175 if $\mathbf{x}_i$ is the brightest firefly

176 Move $\mathbf{x}_i$ randomly and update $I(\mathbf{x}_i)$

177 end if

178 Update I_{best} and x_{best}

179 end for i

180 (3). In every iteration, I_{best} and x_{best} should be recorded. In this step, we update I_{best} and x_{best} according
181 to the best solutions in the last iteration and this iteration.

182 (4). In this study, the condition that judges if the convergence was achieved has been analyzed in the
183 Section 4.3.

184 **4 Experimental Results and Discussion**

185 **4.1 Datasets used for experiments**

186 To evaluate the EE-DFA algorithm proposed in this paper, we applied the proposed algorithm on
187 two series of hyperspectral datasets (synthetic hyperspectral datasets with different SNR and the AVIRIS
188 hyperspectral dataset) for endmember extraction.

189 4.1.1 Synthetic hyperspectral datasets

190 The synthetic hyperspectral image of size 64×64 pixels in this study was created by the six standard
191 spectra (Fig. 2) selected from the United States Geological Survey (USGS) spectral library.

192 First, the six standard spectra (idealized endmembers) were resampled to generate the 10 nm
193 spectral resolution with the 224 spectral bands covering wavelength-range from ~400 nm to ~2500 nm.
194 Second, the whole image (64×64) was divided into units of 8×8 blocks. Pixels in each block were filled
195 up by one spectrum randomly selected from the six standard spectra. To generate a linear mixture, a 9×9
196 averaging filter was applied on the image. Third, to simulate the noise in the data, we add zero-mean
197 Gaussian noise to the mixture image. The covariance matrix of the added noise was defined as a diagonal
198 matrix $\sigma^2 \mathbf{A}$ ($\mathbf{A}$ was an identity matrix). The Signal-to-Noise Ratio (SNR) was defined as follows.

199

$$\text{SNR} = 10 \lg(E[\mathbf{p}^T \mathbf{p}] / E[\boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon}]) \quad (11)$$

200
201
202
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204

$\mathbf{p}$ and $\boldsymbol{\varepsilon}$ represented the spectral signature without noise and the noise of a pixel, respectively. $E[\cdot]$ was the mathematical expectation in spatial dimension. Thus, when the SNR was given, the noise variance was determined by the equation (12).

205
206
207

Fig. 2. Six selected spectra for the synthetic hyperspectral dataset.

$$\sigma^2 = E[\mathbf{p}^T \mathbf{p}] / (10^{\text{SNR}/10} \times L) \quad (12)$$

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The similar creation methods of synthetic hyperspectral datasets were also used in Ref. [15], [30]. To evaluate the impact of different noise levels on EE-DFA method, four synthetic hyperspectral datasets were created with SNR=50 dB, 40 dB, 30 dB, 20 dB, respectively (Fig. 3). Different image quality with different SNR can be easily found from Fig. 3 by visual investigation.

4.1.2 The real hyperspectral image

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The hyperspectral dataset acquired by the AVIRIS sensor over Cuprite, Nevada in the USA, was utilized as the real hyperspectral image to test the proposed method in this study. This dataset has been widely used to test new algorithms of endmember extraction and spectral unmixing in hyperspectral remote sensing [2], [21]. In this paper, a 50-band (1990.8 nm - 2479.0 nm) subset (400×350 pixels) of this dataset is used, which is affiliated to the data resource provided by the ENVI software (filename:

218 “cup95eff.int”). Fig. 4 shows the false color composition of the used subset.

219 In this study, the number of endmembers was determined by a method termed hyperspectral signal
220 identification by minimum error (HySIME). By HySIME, the number of synthetic hyperspectral images
221 and real hyperspectral image was determined as 6 and 8, respectively. The first step of this method is to
222 estimate the signal and noise correlation matrices by multiple regression. Then, the subset of eigenvalues
223 was selected to represent the signal subspace in the sense of least squared error, which is calculated by
224 minimizing the sum of the power of projection error with that of noise. More technical details could be
225 found in Reference [31]. This method has been widely used to determine the intrinsic dimensionality of
226 hyperspectral data (e.g., Reference [32] ~ [35]).

228

229 Fig. 3 Synthetic hyperspectral image with different SNR (Red: 660 nm; Green: 550 nm; Blue: 430 nm)

230

Fig. 4 False color composition of the subset of the AVIRIS Cuprite dataset (Red: Band 183, 2101.0 nm; Green: Band 193, 2200.8 nm; Blue: Band 207, 2340.2 nm).

4.2 Reduction of the calculation complexity

To reduce the calculation complexity, in this study, only a part of the image pixels was used as candidate endmembers to be put in the EE-DFA. The candidate endmembers were selected based convex polyhedron. Under idealized linear condition, the endmembers form a convex simplex in the spectral space and all the image pixels lie inside this simplex, with the endmembers as geometric vertices [36]. Due to some non-linear factors and the noise, some mixed pixels are outside of the simplex, and these outside mixed pixels look like the “vertices” (endmembers) of the simplex. In fact, this is an important reason that impacts the endmember extraction results of SMACC and N-FINDR (Detailed explanation can be found in part C “*Experiments on the synthetic hyperspectral datasets*”). Even so, the real endmembers are still near these “vertices”, and it is highly impossible that the pixels that are far away from these “vertices” are the real endmembers. Hence, in this study, we selected the candidate endmembers from the pixels near the vertices of the simplex.

Here, we give a conceptual explanation on selecting candidate endmembers in 2-dimemensinal spectral space (Fig. 5). In Fig. 5, three points A , C , D , are actually the real endmembers and other black points are the mixed pixels. However, for endmember extraction, we cannot distinguish A , C , D , from the

251 mixed pixels near them, because just by visual investigation, A , C , D , also may be the mixed pixels that
 252 are outside of the simplex (the triangle in 2-dimemensinal spectral space) due to the noise. In other words,
 253 the point B (Fig. 5) is actually a mixed pixels and become outside of the triangle ACD due to the noise.
 254 However, just by visual analysis, B could also be regarded as an endmember, instead of A , and A could
 255 also be regarded as a mixed pixel that are outside of the triangle BCD . Hence, we selected the pixels near
 256 the vertices of the simplex as candidate endmembers. For a relative pure pixel (endmember), the offset
 257 between estimated reflectance and truth reflectance comes primarily from the noise. Given the
 258 probability distribution function of Gaussian distribution, in this study we selected the pixels that obey
 259 following condition as candidate endmembers.

$$|p_{ij} - v_{ij}| < 1.96\sigma \quad (13)$$

260 v_{ij} means the reflectance of the j -th band of the i -th vertice, and p_{ij} means the reflectance of the j -th
 261 band of the candidate pixels near the i -th vertice. All the pixels that obey following condition were
 262 selected as candidate endmembers. For synthetic hyperspectral datasets in this study, the σ was
 263 determined by the equation (12) in the revised manuscript. For AVIRIS dataset, it is shown that the ratio
 264 of signal to noise is $\sim 500:1$ in SWIR band in Reference [37]. The σ was determined by both the equation
 265 (11) and (12). The real endmembers would be determined by EE-DFA method.
 266

267
 268 Fig. 5. Conceptual explanation on selecting candidate endmembers (black points in the red cycles) in
 269 2-dimemensinal spectral space.

271 For hyperspectral dataset with L bands, at first, we used the Minimum Noise Fraction (MNF)
 272 Transform to realize dimensionality reduction. The final dimensionality was determined by the
 273 eigenvalues and the visual quality of the MNF results. In detail, the lowest eigenvalue in the selected
 274 MNF bands should be more than 1 and the last MNF band should visually contain some useful
 275 information of ground surface, not only noise. Then the dimensionality-reduced data were used to
 276 conduct “ n -dimensional visualization” (a function in ENVI software) to select the pixels near the vertices
 277 of the simplex as the candidate endmembers, in which n could be set as the dimensionality reduced in
 278 MNF. In “ n -dimensional visualization”, all the dimensionality-reduced pixels were put in an
 279 n -dimensional space and the pixels near the vertices of the simplex were selected from different
 280 perspectives. In general, the number of real endmembers is much less than that of candidate endmembers.
 281 Then with the number of candidate endmembers increasing, the feasible solutions also increase. So we
 282 set the firefly population size as the number of candidate endmembers in this study.

283 By this way, almost all the pixels that may be real endmembers were selected. The selection steps
 284 are simple, and the result includes dozens of pixels but it is far away from the real endmember extraction
 285 result. Hence, the EE-DFA method is the key process to get the final endmembers. The purpose of this
 286 selection is only to reduce the calculation complexity of the EE-DFA. If we do not select candidate pixels
 287 with the above method, all the image pixels are regarded as the candidate endmembers, and the iteration
 288 times and the number of fireflies should be increased in the EE-DFA method. Candidate endmembers
 289 selection based convex simplex is only one method for selection. In other words, other candidate
 290 endmembers selection methods that can extract almost all the pixels similar to real endmembers, are also
 291 appropriate for the EE-DFA.

292 The computational complexity of EE-DFA was analyzed according to the number of all the cycles in
 293 the procedure. The computational complexities of EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF
 294 are listed in Table 1. In Table 1, k is the iteration times of EE-DFA and MVC-NMF. p is the number of
 295 reduced dimensions in corresponding methods. q is the number of fireflies. N is the number of pixels in
 296 the tested hyperspectral image. M is the maximum iteration times of MVC-NMF the user set. For the
 297 N-FINDR algorithm, the range of η is $2.3 < \eta < 2.9$ [7]. As shown by Fig.7, $k \approx 20$ in the EE-DFA. From the
 298 view of time complexity in the field of software engineering, computational complexities shown by

299 Table 1 are with the polynomial way and belong to same level. What's more, $N \gg p$ and $N \gg q$, so the
 300 computational complexities of are primarily determined by the number of pixels (N). Hence, the
 301 computational complexity of EE-DFA is similar to that of other methods. In consideration of the value of
 302 η (N-FINDR), the complexity of N-FINDR is a little higher than that of other methods and similar
 303 conclusion has been achieved by Reference [7].

304 Table 1. The computational complexities of EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF

Algorithms	Computational Complexity
EE-DFA	$O(k \cdot N \cdot q^2)$
SMACC	$O(p^2 \cdot N)$
N-FINDR	$O(p^{\eta+1} \cdot N)$
VCA	$O(p^2 \cdot N)$
MVC-NMF	$\geq O(50 \cdot k \cdot M)$

305

306 4.3 Parameters analysis and convergence

307 According to the detailed steps of the proposed EE-DFA method (Fig. 1), the parameters to be
 308 analyzed are β_0 , γ , and α . As already mentioned in the “2 Firefly Algorithm (FA)”, β_0 is the attractiveness
 309 at $r_{ij} = 0$. For discrete optimization problem, in general, the movement distance from $\mathbf{x}_i$ to $\mathbf{x}_j$ is less than
 310 $(\mathbf{x}_i - \mathbf{x}_j)$. What's more, if ignoring the tiny randomization step (equation (3)), $\mathbf{x}_i$ should be equal to $\mathbf{x}_j$ after
 311 movement when $r_{ij} = 0$ in discrete optimization problem. Hence, β_0 should be set as 1 in this study.

312 To set the parameters γ and α on the endmember extraction, we conducted experiments of
 313 parametric effect with different values of γ and α using the four synthetic datasets (with different SNR)
 314 and the real hyperspectral dataset (AVIRIS image). The endmember extraction results were evaluated by
 315 the RMSE of spectral unmixing (Fig. 6). For both γ and α , the test range is $[0, 1]$ and the step is 0.1 in the
 316 parameter-effect experiments. In Fig. 6, the RMSE value was linearly interpolated.

317 For different images, the levels of RMSEs are different. To clearly show the locations of minimum
 318 RMSE and then select best ranges of γ and α , we set different scale of RMSE for different images in Fig.
 319 6 because of no need to compare one subfigure of Fig. 6 to another. Fig. 6 indicated that the best ranges of

320 γ and α are $[0.5, 1]$ (γ) and $[0, 0.3]$ (α), respectively, which is also the recommended parametric setting to
 321 the readers. In this parametric range, the results obtained by EE-DFA is steadily better than that with
 322 other parametric setting. We investigated all the experimental results and found that the minimum RMSE
 323 were acquired near $(\gamma, \alpha) = (0.8, 0.1)$. Hence, in subsequent experiments, we set $\gamma=0.8$ and $\alpha=0.1$.

324 Fig. 6 The RMSE with different values of γ and α . (a) RMSE results of 50 dB synthetic hyperspectral dataset; (b)

325 RMSE results of 40 dB synthetic hyperspectral dataset; (c) RMSE results of 30 dB synthetic hyperspectral dataset; (d)
326 RMSE results of 20 dB synthetic hyperspectral dataset; (e) RMSE results of real hyperspectral dataset.

327 Here we give an explanation on the pattern indicated by Fig. 6. The characteristics of convergence
328 and the avoidance from trapping in local optimum are of particular significance for the performance of an
329 optimization algorithm. The parameters γ and α are two important factors in determining the convergence
330 and avoiding trapping in local optimum. As light absorption coefficient, γ characterizes the attractiveness
331 variation of a brighter firefly and determines how FA behaves. In condition where γ tends to zero, the
332 attractiveness is constant and $\beta = \beta_0$. In this case, the attractiveness of a firefly will not decrease with
333 increasing the distance between two fireflies so that x_i will move to the location of x_j directly (equation
334 (3)), and the objective function is easy to achieve local optimum. With increasing the value of γ , the
335 attractiveness of a firefly tends to lower so that the fireflies fly in a more random way, and the objective
336 function is hard to achieve convergence. The contribution of γ are much more than that of α to the
337 convergence, and for the parameter α in firefly algorithm, the original purpose of third term in equation
338 (3) is to add a disturbance to help the objective function escape from local optimum [25, 27]. Since it is a
339 disturbance, the convergence of objective function requests that this disturbance should not be too large,
340 so the value of parameter α should be near zero, but could not equal zero. In this case, to some degree, the
341 value of γ should be away from zero. Hence, the lower value of RMSE presents in the left-up corner in
342 subfigures of Fig. 6. The most arresting pattern is the higher RMSE in the right-up corner in the
343 subfigures of Fig. 6. The higher both γ and α lead to very random behavior of fireflies, and this
344 corresponds to a relative random value of RMSE.

345 In this study, the condition that judges if the convergence of the objective function is achieved is that
346 the iteration times are more than 100 or the updated maximum brightness I_{best} keeps constant in the last
347 three iterations (for one iteration, it starts from “Set $i=1$ ” and ends with the judgement of convergence in
348 Fig. 1). Fig. 7 shows the convergence process of the objective function on the four synthetic datasets and
349 a real dataset in this study, which illustrates that the objective function could achieve the convergence
350 successfully.

Fig. 7 The convergence process of the objective function on the tested datasets

4.4 Comparative experiments on the synthetic hyperspectral datasets

It's unrealistic that all the endmember extraction methods are used for comparative experiments. Hence, we inevitably had to make a selection from these methods, which is the nature of any paper proposing new method. Popular autonomous endmember extraction methods from hyperspectral image mainly include N-FINDR, SMACC, VCA, IEA, ORASIS etc.. The performance of N-FINDR is generally better than ORASIS when SNR is low [7]. VCA projects the image data onto a vector orthogonal to the subspace created by the endmembers already selected, and the advantage of SMACC is that SMACC replaces orthogonal projection by oblique projection to meet the non-negativity restriction of fractional abundance (equation (6)) [7] [8] [38]. IEA is to reach the minimum unmixing error based on pixel by pixel, so the calculation is complicated and IEA is less popular than N-FINDR and SMACC. What's more, it has been shown that SMACC performs better than IEA [8]. MVC-NMF is also a typical method in last recent years [15]. Hence, SMACC, N-FINDR, VCA, and MVC-NMF are selected for comparative experiments in this paper, and all the tested datasets are with their original noise.

Then we conducted experiments on all the four synthetic hyperspectral datasets and the experimental results of the proposed EE-DFA method were compared with those of four typical methods (SMACC, N-FINDR, VCA, and MVC-NMF) (Table 2 to Table 5). The performance of different

endmember extraction methods was evaluated by two parameters: (1) the spectral angles between the extracted endmembers and the ideal endmembers, (2) the RMSE of the spectral unmixing. The definition of spectral angle θ between two spectra is shown in the equation (14), which is same with the calculation in the typical hyperspectral mapping method: Spectral Angle Mapper (SAM) [39] [40].

$$\theta = \arccos \frac{\sum_{i=1}^L S_i T_i}{\sqrt{\sum_{i=1}^L S_i^2 \sum_{i=1}^L T_i^2}}, \theta \in [0, \frac{\pi}{2}] \quad (14)$$

S_i and T_i mean the reflectance of the i -th band of the extracted endmember spectrum and the ideal endmember spectrum, respectively. For the synthetic hyperspectral datasets, the ideal endmembers are the resampled six selected spectra from USGS library. A less spectral angle θ means more similarity between the two spectra.

To analyze the overall performance of different methods, the average of spectral angles from different methods in different SNR situations, was also calculated and shown in Table 2 to Table 5. The spectral angle of “Almandine” in SMACC method is distinctly far from the angles of other materials (SNR=50, 40, 30 dB), which would primarily determine the average. Hence, when calculated the average, we deleted the spectral angle of “Almandine” in SMACC method (please see the “Note” under Table 2 to Table 4). If not, the average of spectral angles would be meaningless. In fact, we found the “Almandine” spectrum in SMACC method with SNR=20 dB was also wrong, but the angle was not distinctly far away from other angles and thus was not deleted when the average was calculated. In all the situations (SNR=50, 40, 30, 20 dB), the average of spectral angles with EE-DFA method is distinctly less than those with SMACC and N-FINDR.

Here, the extracted endmember spectra of the dataset with SNR=40 dB were used as an example for analysis, and were shown in Fig. 8. The comparison between Fig. 2 and Fig. 8 indicated that the endmembers extracted by EE-DFA matched well with the original real endmembers and the differences mainly come from the noise that we added. For the endmembers extracted by SMACC, in fact, the first endmember is similar to Axinite, not Almandine. Hence, two Axinite spectra were extracted by SMACC and this is the reason why the spectral angle of the “Almandine” spectra with SMACC method is abnormal (Table 3). Except the first endmember, other endmembers extracted by SMACC matched well with the original real endmembers (Fig. 2 and Fig. 8). For the endmembers extracted by N-FINDR, the

first endmember is better than that by SMACC. The fifth endmember (Carnallite) is the best one among all the six extracted endmembers (Table 3), and is almost same with that by EE-DFA and N-FINDR. But other four endmembers are worse than those extracted by EE-DFA and N-FINDR.

The endmembers extracted by VCA are similar to those by EE-DFA, but both the spectral angles and the unmixing RMSE with VCA are larger. In terms of the unmixing RMSE, when the SNR =20 dB, the performance of MVC-NMF is better than EE-DFA (Table 5). As the SNR increases, the performance of EE-DFA exceeds other methods including MVC-NMF. When the SNR=30dB, the performance of MVC-NMF is similar to that of EE-DFA (Table 4), and EE-DFA outperforms MVC-NMF when SNR=40 dB and 50 dB. In terms of spectral angles, the performance of EE-DFA is better with SNR=40 dB and 50 dB. When SNR=30 dB, the spectral angles with EE-DFA are also smaller for some materials (e.g., Almandine and Carnallite). In other cases, the MVC-NMF performs better.

Table 2. Comparison of the results of EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF methods on the synthetic hyperspectral dataset (SNR=50 dB)

Materials	EE-DFA	SMACC	N-FINDR	VCA	MVC-NMF
	Spectral Angles (SA)				
Almandine	0.0030	0.3762	0.0031	0.0034	0.0452
Ammonio-Jarosite	0.0030	0.0032	0.0296	0.0031	0.0067
Antigorite	0.0032	0.0033	0.1116	0.0030	0.0128
Axinite	0.0031	0.0032	0.1089	0.0032	0.0247
Biotite	0.0032	0.0031	0.0893	0.0034	0.0193
Carnallite	0.0032	0.0033	0.0033	0.0033	0.0476
Average (SA)	0.00312	0.00322	0.05763	0.00323	0.02605
RMSE	0.0015	0.0083	0.0136	0.0017	0.0053

Note: (The average of spectral angles with SMACC do not include ‘Almandine’)

Table 3. Comparison of the results of EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF methods on the synthetic hyperspectral dataset (SNR=40 dB)

Materials	EE-DFA	SMACC	N-FINDR	VCA	MVC-NMF
	Spectral Angles (SA)				
Almandine	0.0102	0.3774	0.1826	0.0102	0.0452
Ammonio-Jarosite	0.0096	0.0108	0.0575	0.0100	0.0068
Antigorite	0.0102	0.0101	0.2325	0.0103	0.0127
Axinite	0.0103	0.0098	0.1971	0.0109	0.0246
Biotite	0.0099	0.0105	0.0091	0.0109	0.0193

Carnallite	0.0094	0.0103	0.3466	0.0105	0.0476
Average (SA)	0.00993	0.01030	0.17090	0.01047	0.02603
RMSE	0.0047	0.0108	0.0352	0.0048	0.0065

Note: (The average of spectral angles with SMACC do not include ‘Almandine’)

Table 4. Comparison of the results of EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF methods on the synthetic hyperspectral dataset (SNR=30 dB)

Materials	EE-DFA	SMACC	N-FINDR	VCA	MVC-NMF
	Spectral Angles (SA)				
Almandine	0.0304	0.3795	0.1288	0.0325	0.0454
Ammonio-Jarosite	0.0309	0.0292	0.1319	0.0309	0.0070
Antigorite	0.0306	0.0309	0.2548	0.0309	0.0128
Axinite	0.0295	0.0304	0.5395	0.0314	0.0249
Biotite	0.0286	0.0315	0.1404	0.0294	0.0191
Carnallite	0.0298	0.0321	0.0321	0.0321	0.0478
Average (SA)	0.02997	0.03082	0.20458	0.03120	0.02617
RMSE	0.0146	0.0191	0.0514	0.0147	0.0131

Note: (The average of spectral angles with SMACC do not include ‘Almandine’)

Table 5. Comparison of the results of EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF methods on the synthetic hyperspectral dataset (SNR=20 dB)

Materials	EE-DFA	SMACC	N-FINDR	VCA	MVC-NMF
	Spectral Angles (SA)				
Almandine	0.1001	0.3972	0.2296	0.1061	0.0469
Ammonio-Jarosite	0.0988	0.0986	0.1352	0.1081	0.0085
Antigorite	0.1046	0.3895	0.1446	0.1057	0.0124
Axinite	0.1018	0.1021	0.3264	0.1022	0.0243
Biotite	0.0972	0.0995	0.8797	0.1003	0.0197
Carnallite	0.0963	0.1029	0.1029	0.3505	0.0494
Average (SA)	0.09980	0.19830	0.30307	0.14548	0.02687
RMSE	0.0464	0.0565	0.0657	0.0489	0.0375

In detail, for same SNR and material, almost all the spectral angles with EE-DFA are the minimum when compared with SMACC and N-FINDR. Here we use the term “almost”, because only several minimum spectral angles were acquired by SMACC or N-FINDR. Even so, in these unexpected results, the spectral angle with EE-DFA is very close to the minimum value, such as 0.0032 versus 0.0031 (SNR=50 dB, Biotite), 0.0102 versus 0.0101 (SNR=40 dB, Antigorite), 0.0103 versus 0.0098 (SNR=40

425 dB, Axinite), 0.0099 versus 0.0091 (SNR=40 dB, Biotite), 0.0309 versus 0.0292 (SNR=30 dB,
 426 Ammonio-Jarosite), 0.0988 versus 0.0986 (SNR=20 dB, Ammonio-Jarosite). This flaw cannot change
 427 the fact that the performance of EE-DFA evaluated by spectral angle, is distinctly better than that of other
 428 methods.

429
 430 Fig. 8 The extracted endmember spectra of synthetic dataset with SNR=40 dB. (Amm.-Jaro. is the
 431 abbreviation of Ammonio-Jarosite for convenience)
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433 In general, we can approximately regard two spectra as one material when the spectral angle $\theta < 0.1$
 434 rad. For example, the default threshold of SAM method in the ENVI software is exactly 0.1 rad. Most of
 435 spectral angles with the EE-DFA are less than 0.1 rad. The maximum spectral angle with EE-DFA is only
 436 0.1046 rad (“Antigorite”, SNR=20 dB). In this sense, almost all the endmembers extracted by the
 437 EE-DFA method in different SNR situations were correct. However, incorrect identifications were
 438 obviously presented in the results from SMACC and N-FINDR, for example, the “Carnallite” spectrum
 439 with N-FINDR (SNR=40 dB) and all the “Almandine” spectra with SMACC method.

440 Both the RMSE and the average of spectral angles decreases with increasing the SNR, which is
 441 appropriate for all the methods. What’s more, when the noise is high (SNR=20 dB), according to the
 442 spectral angles of different materials, the endmembers were still extracted correctly by EE-DFA, and
 443 EE-DFA has much better performance than other methods. Robustness is important for a proposed

method [41, 42, 43]. This result demonstrates that the proposed EE-DFA method is robust and stable when the noise of the hyperspectral dataset increases sharply, which is different with SMACC and N-FINDR.

Here we give an explanation on the results acquired by EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF. As described in the “1. Introduction”, SMACC, N-FINDR, and VCA are based on a simple geometrical precondition that the endmembers are the vertices of the convex simplex in spectral space. However, due to noise and other non-linear factors, some mixed pixels are outside of the simplex and identified as vertices of the convex simplex by SMACC and N-FINDR. For example, in Fig. 5, the mixed pixel B are outside of the triangle ACD and looks like a vertex of another triangle BCD . The objective of the N-FINDR method is to find the maximum-area (or volume) simplex and the area of the triangle ACD is less than the triangle BCD . Hence, B was regarded as an endmember by N-FINDR and thus the accuracy of endmember extraction by N-FINDR decreased. Similar mechanism is appropriate for the SMACC method. This is the reason why the results of SMACC and N-FINDR are impacted apparently by the SNR. For the proposed EE-DFA, the real endmember A and the mixed pixel B (Fig. 5) can be separated by the RMSE of the spectral unmixing and thus better endmember extraction results can be acquired. Hence, the proposed EE-DFA method is appropriate for non-simplex in spectral space and robust under different SNR. The MVC-NMF method is to calculate the endmember signals, not to identify the relative pure pixels directly. Thus, for the unmixing RMSE, when the SNR is low (SNR=20 dB), the performance of MVC-NMF is better because of the function of removing noise from real pixels. However, as the SNR increases, this advantage of MVC-NMF was not significant, and the performance of EE-DFA becomes the best of all the compared methods.

In above experiments, there are pure pixels in the synthetic datasets. To illustrate the performance of the EE-DFA when there is no pure pixels in the dataset, we fixed the SNR=30dB and generated a dataset without pure pixels. The generating method is similar to the method described in Section 4.1.1. The sole difference is: after a 9×9 averaging filter was applied, we replaced all the pure pixels with mixture pixels that are made up of all endmembers of equal abundances (i.e., in these pixels, the abundance of each endmember equals $1/m$). The experimental results are shown in Table 6. Table 6 suggests that EE-DFA obtained smaller spectral angles and RMSE, and hence the performance of EE-DFA is still better than that of other methods (SMACC, N-FINDR, VCA). The MVC-NMF was designed for highly mixed

image, hence the RMSE with MVC-NMF is less than EE-DFA. But in terms of spectral angles, the performance of EE-DFA is better for some materials (e.g., Almandine and Carnallite).

Table 6 Comparison of the results of EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF methods on the synthetic hyperspectral dataset without pure pixels

Materials	EE-DFA	SMACC	N-FINDR	VCA	MVC-NMF
	Spectral Angles (SA)				
Almandine	0.0295	0.0295	0.2139	0.0517	0.0526
Ammonio-Jarosite	0.0298	0.0411	0.2350	0.0338	0.0073
Antigorite	0.0377	0.0377	0.1315	0.0568	0.0137
Axinite	0.0449	0.0449	0.2237	0.0538	0.0261
Biotite	0.0441	0.0457	0.1709	0.0441	0.0217
Carnallite	0.0369	0.0369	0.0369	0.0523	0.0551
Average (SA)	0.03715	0.03930	0.16865	0.04875	0.02942
RMSE	0.0155	0.0157	0.0473	0.0166	0.0135

4.5 Comparative experiments on the real hyperspectral dataset

The experimental results of the EE-DFA method on the AVIRIS Cuprite dataset were also compared with those of four typical methods (SMACC, N-FINDR, VCA, and MVC-NMF) (Table 7). The spectra of endmember extracted by the four methods and the relevant USGS library spectra are shown in Fig. 9.

Table 7. Comparison of the results of EE-DFA, SMACC, N-FINDR, VCA, and MVC-NMF methods on the real hyperspectral dataset

Materials	EE-DFA	SMACC	N-FINDR	VCA	MVC-NMF
	Spectral Angles (SA)				
Jarosite	0.0306	0.0344	0.0452	0.0928	0.0454
Goethite	0.0519	0.0766	0.0549	0.1229	0.0546
			0.0551		
Palygorskite	0.0527	unknown	0.0559	0.0712	0.0733
Kaolinite	0.0461	0.0581	unknown	0.0805	unknown
Alunite	0.0446	0.0665	0.0564	0.1029	0.0980
Montmorillonite	0.0494	0.0629	0.0511	unknown	0.0787
Calcite	0.0630	0.0778	unknown	0.0832	0.1400
Desert Varnish	0.0554	0.0776	0.0609	0.0746	0.2402
RMSE	0.0041	0.0047	0.0084	0.0090	0.0045

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488 Fig. 9 Spectra from the USGS library and endmembers extracted by EE-DFA, SMACC, N-FINDR,
 489 VCA, and MVC-NMF from the AVIRIS image.

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For the Cuprite AVIRIS subscene, in terms of RMSE, the order of different methods is EE-DFA<SMACC<N-FINDR (Table 7). For both SMACC and N-FINDR, there is an endmember spectrum that cannot be identified, because an abnormal high reflection was presented at approximate 2420 nm (Fig. 9). Moreover, there are two ‘Goethite’ spectra that were extracted as endmembers by N-FINDR. For all the identified endmembers, the spectral angles with EE-DFA method are minimum. In terms of both spectral angles and the unmixing RMSE, EE-DFA outperforms VCA. The unmixing RMSE of MVC-NMF is similar to that of EE-DFA (Table 7). But we investigated the endmember signals calculated by MVC-NMF and found that some of these endmembers are away from standard pure reflectance signals (Table 7 and Fig. 9). The reason is that MVC-NMF calculates new endmember signals to decrease the unmixing error during the iterations, hence the unmixing RMSE is better than those of SMACC, N-FINDR, and VCA.

502 According to both RMSE and spectral angles, the experimental results on the AVIRIS dataset
503 demonstrate that EE-DFA can extracted endmembers successfully from hyperspectral image and is
504 better than the typical popular methods.

505 **5 Conclusions**

506 This paper proposed a novel method named EE-DFA for endmember extraction from hyperspectral
507 image. We redefined the objective function and designed a discretization method for endmember
508 extraction.

509 Here several conclusions were reached. (1) The experiments on both synthetic and real
510 hyperspectral images demonstrate that the endmembers extracted by EE-DFA matched the true/standard
511 spectra better (less spectral angles), compared to the endmembers extracted by existing popular method.
512 (2) EE-DFA reduces the influence from the non-linear factors and the noise, so better spectral unmixing
513 results (less RMSE) can be acquired using the endmembers extracted by the proposed EE-DFA method.
514 (3) The proposed EE-DFA method is robust when the SNR of the image decrease sharply.

515 Although experiments on synthetic hyperspectral datasets with different SNR and AVIRIS image
516 have demonstrated the good performance of the EE-DFA, more hyperspectral datasets should also be
517 used to validate the proposed method further in future research. In addition, for this method, the number
518 of endmembers in the image is one of the inputs. So future work also will focus on improving the
519 EE-DFA to realize endmember extraction without priori knowledge.

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