A New Algorithm for Bilinear Spectral Unmixing of Hyperspectral Images Using Particle Swarm Optimization

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Abstract—Spectral unmixing is an important technique for exploiting hyperspectral data. The presence of nonlinear mixing effects poses an important problem when attempting to provide accurate estimates of the abundance fractions of pure spectral components (endmembers) in a scene. This problem complicates the development of algorithms that can address all types of nonlinear mixtures in the scene. In this paper, we develop a new strategy to simultaneously estimate both the endmember signatures and their corresponding abundances using a biswarm particle swarm optimization (BiPSO) bilinear unmixing technique based on Fan’s model. Our main motivation in this paper is to explore the potential of the newly proposed bilinear mixture model based on particle swarm optimization (PSO) for nonlinear spectral unmixing purposes. By taking advantage of the learning mechanism provided by PSO, we embed a multiobjective optimization technique into the algorithm to handle the more complex constraints in simplex volume minimization algorithms for spectral unmixing, thus avoiding limitations due to penalty factors. Our experimental results, conducted using both synthetic and real hyperspectral data, demonstrate that the proposed BiPSO algorithm can outperform other traditional spectral unmixing techniques by accounting for nonlinearities in the mixtures present in the scene.

Index Terms—Hyperspectral imaging, multiobjective optimization (MO), particle swarm optimization (PSO), simplex volume minimization, spectral unmixing.

I. INTRODUCTION

SPECTRAL unmixing can be considered as a blind signal separating problem that decomposes the pixel observations in a hyperspectral scene into a combination of spectrally pure (endmember) signatures weighted by their corresponding fractional abundances. The linear mixture model (LMM) has been widely applied in spectral unmixing studies [1]. Based on this model, many representative algorithms including the pixel purity index [2], iterative error analysis [3], N-FINDR algorithm [4], and vertex component analysis (VCA) [5] (among others [1]) have been developed to identify endmember signatures for spectral unmixing purposes. These algorithms are based on the assumption that pure pixels (i.e., pixels in which the observation is fully described by a single endmember signature) are present in the scene.

However, due to spatial resolution and other phenomena, it is very likely that hyperspectral scenes may not contain any pure pixels at all. To address this issue, another class of algorithms that do not rely on the pure pixel assumption have been developed. These algorithms aim at solving a minimum simplex volume optimization problem to address the mixed pixel problem when no pure pixels are present in the input scenes [6]. Some representative algorithms of this category include minimum volume transform [7], iterative constrained endmembers (ICE) [8], sparsity-promoting ICE [9], minimum volume transform-nonnegative matrix factorization (NMF) [10], minimum volume simplex analysis [11], and simplex identification via split augmented Lagrangian [12]. Minimum volume algorithms still rely on the LMM, which may not be valid in real scenarios with multiple scattering phenomena, leading to nonlinear mixing effects.

Due to the complex 3-D structure of materials in natural scenes, nonlinear effects still exist even at macroscopic scales. Thus, nonlinear unmixing has become a very important technique for addressing spectral unmixing problems [13]. Many physically inspired nonlinear mixing models (NMMs) have been developed in recent years. For instance, the radiative transfer theory based model (e.g., Hapke’s bidirectional reflectance model [13], [14]) aims to describe photon scattering processes. However, its complex solution of the inherent inverse problem hinders its application for practical applications. As a result, several approximate (but more manageable) NMMs have been developed. A family of bilinear mixing models (bi-LMMs) have received wide interest over the last few years, including the Nascimento model [15], the Fan model (FM) [16], the generalized bilinear model (GBM) [17], the linear-quadratic mixing model [18], and the polynomial post-nonlinear mixing model (PNMM) [19]. These models aim at capturing the most
important nonlinear effects contributed by secondary scattering. Based on the existence of bi-LMMs, developing effective bilinear unmixing algorithms has become a challenge for spectral unmixing algorithms. Many unmixing algorithms including kernel methods [20], [21], semi-NMF algorithm [22], combination of polytope decomposition method with artificial neural network-based learning [23], and constrained least squares algorithms [24] have been presented. However, most unmixing algorithms focus on estimating abundances and assume that the endmembers are known in advance (i.e., these are usually supervised algorithms). To mitigate this dilemma, two strategies have been generally adopted in the literature. One is to develop bi-LMM-based NMF algorithms [25], while the other is to use Bayesian approaches [26].

In this paper, we develop a novel technique for bilinear unmixing of hyperspectral scenes that exploits the concept of swarm intelligence [27]. Specifically, we use a particle swarm optimization (PSO) algorithm, which provides several advantages. First and foremost, the algorithm makes no assumptions about the problem being optimized and does not need any prior information concerning the gradient, Hessian matrix, or probability distributions. As a result, it can be easily applied to characterize complex nonlinear mixtures. Furthermore, unlike classical Lagrange multipliers and penalty function methods, our proposed PSO-based algorithm provides a more flexible mechanism to handle constrained optimization problems, thus avoiding the need to fine tune the penalty factors. In our previous work, we applied the PSO technique successfully to find endmembers based on LMM [28] and to estimate abundances based on the normal compositional model [29], [30] (the latter study also addressed the issue of endmember variability). Our new algorithm has three substantial innovations. First, the new algorithm aims at bilinear unmixing (i.e., based on bi-LMM). Second, the new algorithm is not constrained to the pure pixel assumption because it handles the unmixing task as a nonlinear nonconvex continuous numerical problem instead of a discrete combinational optimization problem. Furthermore, the considered optimization strategies are brand new. For example, our new technique employs a biswarm PSO for bilinear unmixing, exploiting the biswarm mechanism to simultaneously estimate endmembers and abundances. We also use a multiobjective optimization (MO) technique for handling constrained optimization problems.

The remainder of this paper is organized as follows. Section II presents the problem statement. Section III describes the proposed biswarm particle swarm optimization (BiPSO) algorithm. Section IV reports results from both experimental simulations and real data to demonstrate the performance of the proposed algorithm compared with other approaches. Section V concludes the paper with some remarks and hints at plausible future research lines.

II. PROBLEM FORMULATION

A. Nonnegative Matrix Factorization and Convex Geometry Structure

Given a given hyperspectral image with \( N \) pixels, the LMM is simply given by

\[
y[n] = Ey[n] + \varepsilon, \quad n = 1, \ldots, N
\]

where \( y[n] = [y_1[n], \ldots, y_B[n]]^T \), \( n = 1, \ldots, N \) is the \( n \)th pixel vector comprising \( B \) bands, \( E = [e_1, e_2, \ldots, e_M] \in \mathbb{R}^{B \times M} \) is the endmember matrix whose \( i \)th column \( e_i = [e_{i1}, \ldots, e_{iB}]^T \in \mathbb{R}^B \) represents the \( i \)th endmember signature vector, and \( M \) is the total number of endmembers. \( a[n] = [a_1[n], a_2[n], \ldots, a_M[n]]^T \in \mathbb{R}^M \) denotes the abundance fraction for the \( n \)th pixel, and \( \varepsilon \) is a noise vector. The abundance vector generally satisfies two constraints for every \( n = 1, \ldots, N \)

\[
a[n] \geq 0 \quad \text{and} \quad a[n]^T 1 = 1.
\]

Spectral unmixing aims at estimating \( E \) and \( a[n] \) for a given image \( y[n] \), with \( n = 1, \ldots, N \), given the abundance constraints in (2). NMF can be used to solve this problem as follows:

\[
\min_{E \geq 0, a[n] \in \mathbb{R}^M} \sum_{n=1}^{N} \| y[n] - E a[n] \|^2_2
\]

where \( Z = \{ a \in \mathbb{R}^M | a \geq 0, a^T \cdot 1 = 1 \} \).

However, this solution may not be unique [10]. A classical method to solve this problem is to incorporate a convex geometry (CG) structure into the NMF model. Thus, it becomes an optimization problem related with simplex volume minimization, expressed by

\[
\min_{E \geq 0, a[n] \in \mathbb{R}^M} \text{vol}(E)
\]

\[
\text{s.t.} \quad \sum_{n=1}^{N} \| y[n] - E a[n] \|^2_2 \leq \varepsilon,
\]

where \( \text{vol}(E) \) represents the simplex volume measurement determined by the endmembers contained in \( E \). For more details, we refer to [31], [32] and the references therein. Here, we used a measurement based on the sum of the squared distances from the vertices to the centroid [31]. Such a measurement can be expressed as follows:

\[
\text{vol}(E) = \sum_{i=1}^{M} \| e_i - \mathbf{v} \|^2_2
\]

where

\[
\mathbf{v} = \frac{1}{M} \sum_{i=1}^{M} e_i.
\]

B. Bilinear Mixing Model and Unmixing Problem

In this section, we introduce a bilinear term to model the secondary scattering effects between endmembers. The proposed bilinear model can be summarized as

\[
y[n] = E a[n] + n l(E, a[n], \theta) + \varepsilon, \quad n = 1, \ldots, N,
\]

where \( n l(E, a[n], \theta) \) represents the bilinear term, and \( \theta \) is a bilinear parameter. For additional details of the formulation of the bilinear term, we refer to [33]–[35]. Here, we focus on Fan’s model (FM) [16], in which \( \theta \) is omitted and the bilinear term can be simply expressed as follows:

\[
n l(E, a[n]) = \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} a_i[n] a_j[n] e_i \odot e_j.
\]
Thus, the unmixing problem based on a bilinear model can be written as

$$\min_{E \geq 0, a[n] \in Z} \sum_{n=1}^{N} \| y[n] - E a[n] - n l(E, a[n]) \|^2_2.$$  \hspace{1cm} (9)

Analogously to the problem already encountered for the standard NMF formulation above, the solution for (9) may not be unique. Therefore, a CG structure needs to be introduced again so that bilinear unmixing becomes a more complex constrained optimization problem that can be completely formulated as follows:

$$\min_{E \geq 0, a[n] \in Z} \text{vol} (E)$$

$$\text{s.t.} \sum_{n=1}^{N} \| y[n] - E a[n] - n l(E, a[n]) \|^2_2 \leq \varepsilon$$ \hspace{1cm} (10)

Because the objective function and the constraint in (10) are nonconvex, the corresponding optimization process is difficult to handle. Although a nonconvex objective function can be effectively solved by iterative convex approximation [11], [12], the bilinear term becomes an obstacle. Specifically, in these methods, LMM is expressed by $Y = E A$, where $E$ is assumed to be square by using dimensional reduction in advance. The abundance parameters can be eliminated by $A = E^{-1} Y$ for the optimization problem. As a result, they rely on the condition $H = E^{-1}$ to construct a convex approximation. However, in bilm, the abundance parameters are difficult to eliminate due to the nonlinear term. Consequently, the construction of a convex approximation may be complicated. In addition, even if we can find a convex approximation, nonlinear convex optimization still represents a challenge. Another alternative is to apply NMF methods by adding regularization constraints [25]. However, the performance is influenced by regularization parameters such as penalty factors, as mentioned in Section I. Consequently, the regularization parameters must be fine-tuned in practice.

C. Multiobjective Optimization

For the sake of clarity, we highlight the aforementioned problem from a MO viewpoint. In MO, the problem in (10) can be decomposed into two objective functions. Let $A = \{a[n]\}_{n=1}^{N}$ and

$$f_1 (E, A) = \sum_{n=1}^{N} \| y[n] - E a[n] - n l(E, a[n]) \|^2_2$$ \hspace{1cm} (11)

$$f_2 (E) = \text{vol} (E).$$ \hspace{1cm} (12)

The function value of $f_1$ can be interpreted as the nonlinear reconstruction error (NRE) for the estimation of parameters $E$ and $A$.

Fig. 1 graphically illustrates the objective function space of the proposed method. In MO, the problem in (10) can be completely formulated as follows:

$$\min_{E \geq 0, a[n] \in Z} \text{vol} (E)$$

$$\text{s.t.} \sum_{n=1}^{N} \| y[n] - E a[n] - n l(E, a[n]) \|^2_2 \leq \varepsilon$$ \hspace{1cm} (10)

Because the objective function and the constraint in (10) are nonconvex, the corresponding optimization process is difficult to handle. Although a nonconvex objective function can be effectively solved by iterative convex approximation [11], [12], the bilinear term becomes an obstacle. Specifically, in these methods, LMM is expressed by $Y = E A$, where $E$ is assumed to be square by using dimensional reduction in advance. The abundance parameters can be eliminated by $A = E^{-1} Y$ for the optimization problem. As a result, they rely on the condition $H = E^{-1}$ to construct a convex approximation. However, in bilm, the abundance parameters are difficult to eliminate due to the nonlinear term. Consequently, the construction of a convex approximation may be complicated. In addition, even if we can find a convex approximation, nonlinear convex optimization still represents a challenge. Another alternative is to apply NMF methods by adding regularization constraints [25]. However, the performance is influenced by regularization parameters such as penalty factors, as mentioned in Section I. Consequently, the regularization parameters must be fine-tuned in practice.

III. BILINEAR UNMIXING PARTICLE SWARM OPTIMIZATION ALGORITHM

In this section, we develop a biswarm PSO bilinear unmixing algorithm to solve the spectral unmixing problem. After briefly reviewing the standard PSO solutions, we describe a biswarm mechanism for simultaneously estimating the spectral endmembers and their corresponding fractional abundances. Then, we introduce a MO technique to specifically solve the constrained optimization problem in (10). Furthermore, to make our algorithm more suitable for hyperspectral images, we develop a strategy to extend the algorithm to high-dimensional data. This section concludes with a complete algorithmic description of the proposed method.

A. Standard Particle Swarm Optimization Algorithm

PSO is a population-based optimization technique, in which the population is called a swarm. Each particle in the swarm represents a possible solution to the optimization problem. Specifically, each particle $i$ has its own current position $X_i$, current velocity $V_i$, and a personal best position $P_i$ in the search space, where $1 \leq i \leq s$ and $s$ is the size of the swarm (i.e., the number of particles).

Let $f$ denote the objective function. PSO adopts an iterative procedure in which, at each step, it performs the so-called moving and updating operations alternately. Specifically, the operations at time step $j$ can be summarized as follows. In the moving
operation, the velocity of particle is determined by
\[
V^{(j+1)}_i = wV^{(j)}_i + c_1 r_1^{(j)} (P^{(j)}_i - X^{(j)}_i) + c_2 r_2^{(j)} (G^{(j)} - X^{(j)}_i)
\]  
(13)
for all \(i \in 1, \ldots, s\), where \(w\) is an inertial weight that varies linearly from 1 to near 0 during the course of PSO optimization. Similarly, \(c_1\) and \(c_2\) denote the acceleration coefficients; \(r_1\) and \(r_2\) are elements from two uniform random sequences in the range \((0, 1)\), and \(G\) represents the global best position selected from \(P_i\), \(1 \leq i \leq s\) in the current step. The particles move according to
\[
X^{(j+1)}_i = X^{(j)}_i + V^{(j+1)}_i.
\]  
(14)
The updating operation works as follows. First, the personal best position of each particle is updated using
\[
P^{(j+1)}_i = \begin{cases} 
P^{(j)}_i, & \text{if } f(X^{(j+1)}_i) \geq f(P^{(j)}_i) \\
X^{(j+1)}_i, & \text{if } f(X^{(j+1)}_i) < f(P^{(j)}_i)
\end{cases}.
\]  
(15)
Subsequently, the global best particle is updated by
\[
G^{(j+1)} = \arg \min_{P^{(j+1)}} \left\{ f(P^{(j+1)}_i, \text{for all } i \in 1, \ldots, s) \right\}.
\]  
(16)
These operations are repeated until a termination criterion (e.g., a predefined number of iterations \(i_{\text{end}}\)) is met. At this point, PSO yields a final solution \(G^{(i_{\text{end}})}\).

We can see that PSO employs a fitness value that is determined directly by the objective function. Thus, the computation is very simple and can be easily implemented for nonlinear unmixing compared to gradients or a Hessian matrix. Indeed, in many applications [36]–[45], PSO has demonstrated its capacity to solve both nonlinear and nonconvex optimization problems. In this paper, we have used PSO to solve problem (10). Furthermore, the operations performed by PSO provide a feasible mechanism for employing multiobjective techniques to avoid fine-tuning penalty factors, an aspect that will be discussed in detail in Section C.

**B. Biswarm Mechanism for Endmember Identification and Abundance Estimation**

Considering problem (10), the endmembers \(E\) and the corresponding abundances \(A\) need to be estimated. Because problem (10) is nonlinear, the traditional least squares method is not appropriate in this context. Let us denote the swarm for endmembers estimation by SE and the swarm for abundances estimation by SA. Our algorithm finds a solution by alternately minimizing the objective function in accordance with the two aforementioned swarms as follows. For brevity, we denote the optimization problem (10) as a formulation of \(OP(E, A)\) with respect to two groups of parameter sets: \(A\) and \(E\). The procedure is illustrated in Fig. 2. At the \(t\)th step, SE particles update their velocities and move to subsequent positions. As a result, the personal best position of the particles and the global best particle can be updated by evaluating \(OP(E, A)\) with their positions as \(E\), while another parameter set \(A\) is fixed to the position of the global best particle of SA at the current step (we denote this as \(G_A\)). After the SE has finished the updating operation, it stops and waits. Then, the SA begins to perform its moving and updating operations. At this point, the global best particle of the SE (denoted as \(G_E\)) is used as a fixed parameter of \(E\) in \(OP(E, A)\). The SE and the SA repeat this procedure alternately so that the two swarms share and exchange their global best positions. As a consequence, the swarms guide each other in the correct direction.
C. MultiObjective Optimization

Recently, many studies have successfully solved constrained optimization problems by combining evolutionary optimization with multiobjective techniques [46]–[49]. For example, CMODE [47] used differential evolutionary strategies as the search engine and demonstrated competitive performance based on MO. In this section, we adopt the idea behind this method into our biswarm PSO algorithm. Specifically, our method uses two performance indicators to measure the quality of particles instead of the objective function value. The first indicator treats the problem as a MO problem and uses Pareto dominance to evaluate the particles. Another indicator considers the feasibility of the particles and introduces a feasibility-based rule to compare the particles. We slightly simplify the computation as follows. To be consistent with the standard PSO formulation, we use the notations \( X, P_i \), and \( G \), which represent (for the SE) the estimation of parameter \( E \). According to the concept of Pareto dominance, a particle \( X_i \) is said to Pareto dominate another particle \( X_j \) if it satisfies

\[
\forall k \in \{1, 2\}, f_k (X_j^{(j+1)}) \leq f_k (X_i^{(j+1)})
\]

and

\[
\exists k \in \{1, 2\}, f_k (X_i^{(j+1)}) < f_k (X_j^{(j+1)})
\]

where \( f_1 \) and \( f_2 \) are defined in (11) and (12), respectively. Let us denote the Pareto dominance number by a particle \( X_i \) as

\[
\text{pd}(X_i) = \text{card} \{X_j \mid \forall X_j \in \text{SE and } X_i \text{ Pareto dominates } X_j \}
\]

(18)

where \( \text{card} \{\cdot\} \) is the cardinality of the set. Thus, the final indicator function can be written as

\[
u(X_i) = \begin{cases} 
\text{order}(X_i, \text{pd}, S, 'D') & X_i \in S \\
\text{n}_s + \text{order}(X_i, \text{pd}, \overset{\cdot}{S}, 'D') & X_i \in \overset{\cdot}{S}
\end{cases}
\]

(19)

where \( S \) is the set of feasible particles and \( \overset{\cdot}{S} \) corresponds to the set of infeasible particles, \( n_s \) is the cardinality of \( S \), and \( \text{order}(X_i, \text{pd}, \cdot, 'D') \) represents the sequence number of particle \( X_i \), which is sorted in descending order according to the value of \( \text{pd} \) with respect to \( X \) in the \( \cdot \) set. The indicator function shows that the particles are arranged in a sequence according to the two main criteria: a) the particles with higher \( \text{pd} \) values are listed in front of those with lower \( \text{pd} \) values, and b) feasible particles are listed in front of infeasible particles.

D. High-Dimensional Extension

An important drawback of PSO algorithms is that they can be applied only to a search space with a fixed and low dimension. However, bilinear unmixing for hyperspectral images is a high-dimensional optimization problem due to the dimensionality of the image data. Many strategies have been proposed to improve the high-dimensional searching capabilities of PSO algorithms [50]–[52]. Based on these works, we develop a strategy for a high-dimensional extension of the SE in our particular case as follows. Considering (11) and (12) in the \( k \)th dimension, the optimization subproblem can be written as

\[
f_{1,k}(E, A) = \sum_{n=1}^{N} \|y_k[n] - E_k a[n] - nl(E_k, a[n])\|^2_2
\]

(20)

\[
f_{2,k}(E) = \text{vol}(E_k)
\]

(21)

where symbol \( E_k \) represents the \( k \)th row of \( E \) and

\[
nl(E_k, a[n]) = \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} a_i[n] a_j[n] e_{k,i} e_{k,j}
\]

(22)

\[
\text{vol}(E_k) = \sum_{i=1}^{M} (e_{k,i} - \bar{e}_k)^2
\]

(23)

\[
\bar{e}_k = \frac{1}{M} \sum_{i=1}^{M} e_{k,i}
\]

(24)

We denote \( f_{1,k}(E, A) \) and \( f_{2,k}(E) \) by \( f_1, k \) and \( f_2, k \), respectively, to simplify the notation. Thus, the objective function can be separated and rewritten in the \( B \)-dimensional objective vector form

\[
f_1 = [f_{1,1}, f_{1,2}, \ldots, f_{1,B}]^T \text{ and } f_2 = [f_{2,1}, f_{2,2}, \ldots, f_{2,B}]^T.
\]

(25)

Then, we replace the objective functions presented in (11) and (12) with the objective vectors mentioned above and calculated by (17)–(19) separately in each dimension. Eventually, we obtain the following \( B \)-dimensional indicator

\[
u(X_i) = [u_1(X_i), u_2(X_i), \ldots, u_B(X_i)]^T, i = 1, \ldots, s
\]

(26)

where \( u_k(X_i) \) represents an indicator in the \( k \)th dimension of particle \( X_i \). Based on the \( B \)-dimensional indicator, the updating operation becomes

\[
P_{i}^{(j+1)} = \left[ P_{i,1}^{(j+1)} P_{i,2}^{(j+1)} \cdots P_{i,B}^{(j+1)} \right]^T
\]

(27)

where each component is now obtained by

\[
P_{i,k}^{(j+1)} = \begin{cases} 
P_k^{(j)} & \text{if } u_k(X_i^{(j+1)}) \geq u_k(P_k^{(j)}) \\
x_k^{(j)} & \text{if } u_k(X_i^{(j+1)}) < u_k(P_k^{(j)})
\end{cases}
\]

(28)

where \( (\cdot)_k \) represents the \( k \)th row of the matrix \( \cdot \).

Then, the global best particle can be updated by

\[
G_{E}^{(j+1)} = \left[ G_{E,1}^{(j+1)} G_{E,2}^{(j+1)} \cdots G_{E,B}^{(j+1)} \right]^T
\]

(29)

where each component is given by

\[
G_{E,k}^{(j+1)} = \arg \min_{P_k^{(j+1)} \in \text{SE}} \left\{ u_k(P_k^{(j+1)}) \right\}_k
\]

(30)

Note that (28) can take advantage of the available diversity among individual dimensional components, and thus prevent the swarm from being trapped in local optima. With the aforementioned considerations in mind, Table I summarizes the proposed BiPSO bilinear unmixing algorithm.

It is worth noting that, on one hand, the proposed method cannot guarantee the global convergence property because it is
the GBM can be applied in our experiments. We also used two state-of-the-art supervised algorithms: constrained nonlinear least squares algorithm (CNLS) and an optimized version of an unmixing algorithm for the kernel-based hyperspectral mixture model (SK-Hype). The second group of algorithms contains a nonnegative matrix factorization method for spectral unmixing based on the FM [25] (denoted by Fan-NMF), which can provide the endmembers and the abundances simultaneously. We did not impose volume constraints in our implementation on Fan-NMF, but we used the VCA algorithm for initialization. The third group also contains the two different versions of PSO, i.e., the single swarm PSO algorithm (see Section B), and the LMM-based PSO algorithm (denoted by linear PSO), where the FM is replaced by LMM.

All algorithms were run on the same computing environment: an Intel Core i5-3570 CPU (3.4 GHz, 4 cores) with 16 GB of memory. The endmember spectra and abundance fractions were initialized by the VCA and the fully constrained least square algorithm [58], respectively, for all algorithms. To obtain robust results for the algorithms, all algorithms were run for a maximum of 500 iterations. The convergence tolerance threshold was set empirically to $10^{-6}$.

In our performance comparison, each algorithm was run ten times for each considered dataset, and their average scores are reported. Four performance measures were used. The execution time was recorded to compare the computational cost of the algorithms. The average spectral angle distance (SAD) [59] was computed to evaluate the accuracy of endmember identification. The accuracy of abundance estimation and the overall accuracy can be evaluated by the average abundance error (AAE) and average reconstruction error (ARE), respectively, as follows:

$$\text{AAE} = \sqrt{\frac{1}{NM} \sum_{n=1}^{N} \left( \mathbf{a} \left[ n \right] - \hat{\mathbf{a}} \left[ n \right] \right)^2}$$

$$\text{ARE} = \sqrt{\frac{1}{NB} \sum_{n=1}^{N} \left( \mathbf{y} \left[ n \right] - \hat{\mathbf{y}} \left[ n \right] \right)^2}.$$  

### A. Parameter Configuration and Sensitivity Analysis on Swarm Size

In the proposed algorithm, the inertia weight was calculated by the linear descent algorithm according to [60]–[62]

$$w \left( t \right) = \left( w \left( 0 \right) - w \left( t_{\text{max}} \right) \right) \frac{t_{\text{max}} - t}{t_{\text{max}}} + w \left( t_{\text{max}} \right)$$  

where $w \left( t \right) = 0.9$ represents the weight in the $t$th iteration, $w \left( 0 \right) = 0.4$ represents the initial weight, and $w \left( t_{\text{max}} \right)$ is the weight in the final iteration, i.e., $t_{\text{max}}$.

The acceleration coefficients were obtained as follows [62]:

$$c_1 \left( t \right) = \left( 0.5 - 2.5 \right) t_{\text{max}} + 2.5$$

$$c_2 \left( t \right) = \left( 2.5 - 0.5 \right) t_{\text{max}} + 0.5.$$  

The swarm size is a problem-specific parameter in the PSO algorithm. Considering (10), the problem size depends on the number of endmembers $M$ and the number of pixels $N$. The sensitivity of the swarm size with respect to these factors is shown in Figs. 3 and 4, respectively. Fig. 3 compares the sensitivity as the number of endmembers varied from 3 to 7. The curves
Fig. 3. Swarm size sensitivity curves for different numbers of endmembers \((M = 3, 5, \text{ and } 7)\), where \(F\) represents the final value of the objective function obtained by the proposal algorithm, and \(F_{\text{global}}\) represents the value of the global optimal solution (i.e., true endmembers and abundances).

Fig. 4. Swarm size sensitivity curves for different numbers of pixels \((N = 500, 1000, \text{ and } 2000)\).

Fig. 5. USGS library spectra of the five endmembers used in our synthetic data experiments.

The performance increases as the swarm size increases. As shown in Fig. 3, when the size reaches a stable point (e.g., 15 particles for \(M = 3\)), small improvements will be obtained as we continue to increase the size. This means that the stable point is a suitable size for use in the algorithm. By comparing these curves, we can see that the stable point varies with respect to the number of endmembers. Specifically, as the number of endmembers increases, we need to increase the swarm size (to reach a stable point). Fig. 4 compares the sensitivity of the swarm size with respect to the number of pixels. These curves had similar trade and stable point, which indicates that the sensitivity of the swarm size is not obviously affected by the image size variations.

In practice, we can evaluate the performance using simulations to determine the suitable size. It is not critical to select the exact stable point, but it is necessary to guarantee that the swarm size is not smaller than the stable point (a greater swarm size does not reduce the performance but merely costs more computational time). Empirically, we respectively use 20, 30, and 35 particles for three, five, and seven endmembers in the algorithm. We use 30 particles in the following experiments.

indicate that the performance increases as the swarm size increases. As shown in Fig. 3, when the size reaches a stable point (e.g., 15 particles for \(M = 3\)), small improvements will be obtained as we continue to increase the size. This means that the stable point is a suitable size for use in the algorithm. By comparing these curves, we can see that the stable point varies with respect to the number of endmembers. Specifically, as the number of endmembers increases, we need to increase the swarm size (to reach a stable point). Fig. 4 compares the sensitivity of the swarm size with respect to the number of pixels. These curves had similar trade and stable point, which indicates that the sensitivity of the swarm size is not obviously affected by the image size variations.

In practice, we can evaluate the performance using simulations to determine the suitable size. It is not critical to select the exact stable point, but it is necessary to guarantee that the swarm size is not smaller than the stable point (a greater swarm size does not reduce the performance but merely costs more computational time). Empirically, we respectively use 20, 30, and 35 particles for three, five, and seven endmembers in the algorithm. We use 30 particles in the following experiments.

<table>
<thead>
<tr>
<th>Algorithms</th>
<th>SAD (RADIANS), AAE, ARE scores ((\times 10^{-2})), and Execution Time of Single Swarm and Biswarm PSO for the Synthetic Dataset with 40 dB SNRs and Maximum Purity Levels of 0.8</th>
</tr>
</thead>
</table>
| Algosn SADF| \begin{tabular}{lrrrr} 
| Single Swarm & 0.114 & 0.380 & 34.50 & 21225.1 \\
| Biswarm      & 0.033 & 0.062 & 0.664 & 101.318 \\
\end{tabular} |

<table>
<thead>
<tr>
<th>TABLE III</th>
<th>Time Percentages for the Main Operations Involved in the Algorithms</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single Swarm</td>
<td>Biswarm</td>
</tr>
<tr>
<td>Operation Time percentage (100%)</td>
<td>Operation Time percentage (100%)</td>
</tr>
<tr>
<td>CNLS 99.61725</td>
<td>-</td>
</tr>
<tr>
<td>Move(SE) 0.067746</td>
<td>Move(SE + SA) 8.122156</td>
</tr>
<tr>
<td>Update(SE) 0.297024</td>
<td>Update(SE + SA) 82.41656</td>
</tr>
<tr>
<td>Other 0.017505</td>
<td>Other 9.466199</td>
</tr>
</tbody>
</table>

B. Comparison between Single Swarm and Biswarm

We generated synthetic hyperspectral dataset composed of \(N = 1000\) pixels and 224 bands using the FM [16], [18]. Five endmembers (see Fig. 5) were selected from the United States Geological Survey (USGS) spectral library [63], including maple tree leaves, dry grass, and three randomly selected minerals, i.e., olivine, calcite, and quartz. Their abundance fractions were generated following a Dirichlet distribution [5]. The first group of synthetic scenes was created with maximum endmember purity levels \(\rho = 0.8\) and with zero-mean Gaussian noise added at a 40 dB signal-to-noise ratio (SNR).

We also developed a single swarm version PSO that replaces SA with one of the fastest unmixing algorithms (i.e., the CNLS algorithm) for abundance estimation in each iteration. The results listed in Table II show that using the biswarm greatly improves the performance of PSO. Table III reveals that abundance estimation (CNLS) occupied the majority of time in single swarm PSO compared to other operations. Although the CNLS algorithm is very fast, it executes hundreds of times during the
iterations. Consequently, the overall time consumed was more than 5 h. Conversely, in the biswarm framework, the computations related to the moving and updating operations in SE and SA are simple compared to the CNLS algorithm, which reduced the overall time to only several minutes.

C. Experiments With Various Endmember Purity Levels and SNRs

The second group of synthetic scenes was created with maximum endmember purity levels ranging from 0.6 to 0.9 and with zero-mean Gaussian noise added at different SNRs varying from 20 to 50 dB. Fig. 6 compares the convergence curves between BiPSO and Fan-NMF in the case with 30 dB SNRs and a maximum endmember purity level of 0.8. The BiPSO had a similar overall convergence as Fan-NMF. In detail, Fan-NMF had slightly better convergence before the first 200 iterations, but the performance of BiPSO was very similar. After 200 iterations, BiPSO obtains slightly better values.

Tables IV and V further compare the results in terms of the SAD, AAE, and ARE metrics and the execution time for the compared algorithms on the synthetic data. Regarding endmember estimation performance, BiPSO outperformed the other algorithms. In particular, when $\rho \geq 0.7$, the BiPSO scheme delivered good performance in terms of endmember estimation and higher robustness against SNRs. With $\rho = 0.6$, the performances of all the tested algorithms were significantly degraded. This occurs primarily because, at this level, the solution may be ambiguous due to the low purity present in the simulated mixtures. Fan-NMF obtains better endmember estimation results than VCA. In terms of abundance estimation performance, BiPSO was more robust than the other tested algorithms, even in low SNR conditions. As a result, BiPSO presented a lower ARE score than the other algorithms. Furthermore, it should be noted that the ARE scores of Fan-NMF and BiPSO were close at a 20 dB SNR, but BiPSO had lower SAD and AAE scores. This suggests that Fan-NMF became trapped in a local optimal solution while BiPSO provided a better overall solution. In addition, we can also see that the performances of GBA, CNLS, and SK-Hype were limited by the pure pixel requirement, which is necessary for VCA to perform endmember identification properly. Comparing linear PSO and BiPSO, linear PSO had an ARE score similar to BiPSO at low SNR (20 dB) levels but had larger ARE scores in other cases. Furthermore, linear PSO had larger SAD and AAE scores than BiPSO. Specifically, it gained an average of 37.70% in terms of SAD and 27% in terms of AAE with $\rho = 0.6$, while it gained 114.3%, 280.3%, and 174.6% in terms of SAD and 151.4%, 160.4%, and 203.7% in terms of AAE when $\rho = 0.7$, 0.8, and 0.9, respectively. This result indicates that the traditional LMM has significant errors when using the FM.

Regarding execution time, BiPSO cost approximately 100 s and was approximately equal to Fan-NMF—or even faster in some cases. Furthermore, BiPSO and Fan-NMF were slower than the GBA, CNLS, and SK-Hype algorithms because the latter did not consider endmember estimation. Linear PSO achieved a better execution time than BiPSO because the calculation of LMM in linear PSO is simpler than the calculation of bi-LMM. However, linear PSO is subject to the model-mismatching problem.

D. Experiments With Different Bilinear Mixing Models

The third group of synthetic scenes was created by using GBM and PPNMM, respectively, with zero-mean Gaussian noise at a 40 dB SNR and a maximum purity level of 0.8. The nonlinearity coefficients for GBM were uniformly drawn from the range $[0, 1]$, while the amplitude parameter for PPNMM was uniformly generated in a range of $[-0.3, 0.3]$ as in [19]. Table VI lists the performance results of these five algorithms. It is worth noting that the ARE results for VCA/SK-Hype can only be estimated because SK-Hype delivers only an estimation of the abundance parameters. Thus, the ARE results for VCA/SK-Hype were obtained by using the FM to recover the reconstructed image.

For GBM, the endmember estimation performances achieved by BiPSO and Fan-NMF were better than VCA, and the abundance estimation performance achieved by BiPSO was better than other algorithms, indicating that BiPSO can be suitable for unmixing GBM. BiPSO outperformed the other methods in terms of endmember detection but suffered from model mismatch issues when the abundance estimation and reconstruction error were considered. Linear PSO obtained lower ARE scores than BiPSO, while the endmember and abundance estimation performance obtained by BiPSO were better than linear PSO. This result indicates that although the LMM obtained a better overall error score, it still obtains significant errors for GBM. The performance of the supervised algorithms was still limited by the purity pixel requirement even though the models were exactly matched (e.g., GBA for GBM). Among these supervised algorithms, SK-Hype demonstrated better performance in terms of SAD, AAE, and computational cost. The same trend behavior for supervised algorithms can be observed for the PPNMM-based scene.

In details, Table VI shows that BiPSO provides good performance in terms of both endmember detection and abundance estimation on GBM-based scenes. Specifically, BiPSO is able to efficiently track the nonlinearities induced by the second-order nonlinear interplay between the endmembers and the quadratic terms in the dataset generated according to GBM. Indeed, comparing BiPSO to the second-best unmixing method performance
### TABLE IV

<table>
<thead>
<tr>
<th>Image Parameters</th>
<th>SNR(dB)</th>
<th>20</th>
<th>30</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SAD</td>
<td>AAE</td>
<td>ARE</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>SAD (RADIANS), AAE, ARE ((10^{-2})) SCORES, AND EXECUTION TIMES OF SIX DIFFERENT SPECTRAL UNMIXING ALGORITHMS FOR THE SYNTHETIC DATASET WITH SNRS VARYING FROM 20 TO 30 dB AND MAXIMUM PURITY LEVELS (FROM 0.6 TO 0.9)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BiPSO</td>
<td>0.6</td>
<td>0.103</td>
<td>0.147</td>
</tr>
<tr>
<td></td>
<td>0.7</td>
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<td>0.6</td>
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<td>0.223</td>
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<td>0.094</td>
<td>0.18</td>
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<td>0.9</td>
<td>0.067</td>
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<td>0.067</td>
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<tr>
<td>LinearPSO</td>
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<td>0.229</td>
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<td></td>
<td>0.7</td>
<td>0.133</td>
<td>0.217</td>
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<td>0.8</td>
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<td>0.066</td>
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### TABLE V

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<th>Image parameters</th>
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<td>ARE</td>
</tr>
<tr>
<td></td>
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<tr>
<td><strong>SAD (RADIANS), AAE, ARE ((10^{-2})) SCORES, AND EXECUTION TIMES OF SIX DIFFERENT SPECTRAL UNMIXING ALGORITHMS FOR THE SYNTHETIC DATASET WITH SNRS VARYING FROM 40 TO 50 dB AND MAXIMUM PURITY LEVELS (FROM 0.6 TO 0.9)</strong></td>
<td></td>
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<tr>
<td>BiPSO</td>
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<td>0.07</td>
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<tr>
<td>VCA/SK-Hype</td>
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<td>0.046</td>
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<tr>
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TABLE VI
SAD (RADIANS), AAE, ARE ($\times 10^{-4}$) SCORES, AND EXECUTION TIMES OF SIX DIFFERENT SPECTRAL UNMIXING ALGORITHMS FOR THE SYNTHETIC DATASET USING GBM AND PPNMM

<table>
<thead>
<tr>
<th>Algorithms</th>
<th>GBM</th>
<th>PPNMM</th>
</tr>
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<td>Fan-NMF</td>
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<tr>
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<td>VCA/CNLS</td>
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<td>0.098</td>
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<tr>
<td>VCA/SK-Hype</td>
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<td>0.059</td>
</tr>
<tr>
<td>Linear PSO</td>
<td>0.114</td>
<td>0.124</td>
</tr>
</tbody>
</table>

*Note: the ARE values of SK-Hype were estimated by employing the FM for reconstruction (we cannot obtain other bilinear parameters from SK-Hype).

(23), the SE objective function can be decomposed in the endmembers’ cross-contributions according to the binomial theorem [65]. Therefore, BiPSO can still track the nonlinear effects that the quadratic contributions in PPNMM confer on the dataset (i.e., the proposed method achieves good performance in terms of SAD). Consequently, the nonlinear optimization performed by BiPSO is still able to track the quadratic contributions in PPNMM on the vertices of the data hull, allowing BiPSO to outperform the other nonlinear algorithms when identifying endmembers. Linear PSO obtained ARE scores similar to those of BiPSO, while the endmember and abundance estimation performances achieved by BiPSO were better than those of linear PSO—which again indicates that linear PSO is not suitable for nonlinear models.

However, the swarm optimization approach effectively overcomes the model mismatch during endmember identification: BiPSO delivers a 15.79% gain in terms of SAD with respect to the second-best performing algorithm. Indeed, when detecting endmembers, the trajectory drift provided by the difference between PPNMM and the FM used by BiPSO is leveraged because the biswarm search focuses on the geometric volume optimization of the data cloud [64]. Thus, as the swarm for endmember estimation relies on the aggregate metric in (5) and (23), the SE objective function can be decomposed in the endmembers’ cross-contributions according to the binomial theorem [65]. Therefore, BiPSO can still track the nonlinear effects that the quadratic contributions in PPNMM confer on the dataset (i.e., the proposed method achieves good performance in terms of SAD). Consequently, the nonlinear optimization performed by BiPSO is still able to track the quadratic contributions in PPNMM on the vertices of the data hull, allowing BiPSO to outperform the other nonlinear algorithms when identifying endmembers. Linear PSO obtained ARE scores similar to those of BiPSO, while the endmember and abundance estimation performances achieved by BiPSO were better than those of linear PSO—which again indicates that linear PSO is not suitable for nonlinear models.

Hence, BiPSO represents a valid option for describing and characterizing scenes that show bilinear interactions between endmembers. Moreover, the proposed scheme can be used to detect the endmembers in images where the nonlinear effects are provided only by quadratic nonlinear contributions, although it can hardly provide accurate details when evaluating abundance maps. Considering the execution time, BiPSO was faster than Fan-NMF and approximately equal to linear PSO. This indicates that the search capability of BiPSO is better than the traditional NMF algorithm in different bi-LMM cases. Furthermore, although the model calculation in linear PSO is simple, it spent much time matching data to LMM in these cases. Thus, linear PSO has an execution time similar to BiPSO.

E. Experiments Using Real Hyperspectral Data

We also evaluated the performance of the considered spectral unmixing algorithms using two real hyperspectral images.

The first scene [66] was acquired in 1997 by the airborne visible infrared imaging spectrometer (AVIRIS) over Moffett Field (CA, USA). A subimage of size $50 \times 50$ pixels was chosen for our experiments. We selected this subscene because it has been widely used in spectral unmixing literature [17], [25]. After removing bands 1–7, 108–113, 152–169, and 221–224 due to water absorption and low SNR in those bands, 189 bands were used. Water, vegetation, and soil constituted three main materials in the scene. We ran the different algorithms by separately. Thus, the FM employed by BiPSO can only drive the optimization process towards local minima within the search space [65]. Hence, the BiPSO optimization trajectory apparently cannot efficiently counteract and recover the deviation induced by the mismatch between PPNMM and FM on the proposed iterative scheme, because the cross-term nonlinear effects considered in BiPSO mislead the search orbit. This process causes the performance loss that BiPSO delivers with respect to the best performing algorithm on the PPNMM-generated dataset (i.e., 33.77% in AAE).

However, the swarm optimization approach effectively overcomes the model mismatch during endmember identification: BiPSO delivers a 15.79% gain in terms of SAD with respect to the second-best performing algorithm. Indeed, when detecting endmembers, the trajectory drift provided by the difference between PPNMM and the FM used by BiPSO is leveraged because the biswarm search focuses on the geometric volume optimization of the data cloud [64]. Thus, as the swarm for endmember estimation relies on the aggregate metric in (5) and (23), the SE objective function can be decomposed in the endmembers’ cross-contributions according to the binomial theorem [65]. Therefore, BiPSO can still track the nonlinear effects that the quadratic contributions in PPNMM confer on the dataset (i.e., the proposed method achieves good performance in terms of SAD). Consequently, the nonlinear optimization performed by BiPSO is still able to track the quadratic contributions in PPNMM on the vertices of the data hull, allowing BiPSO to outperform the other nonlinear algorithms when identifying endmembers. Linear PSO obtained ARE scores similar to those of BiPSO, while the endmember and abundance estimation performances achieved by BiPSO were better than those of linear PSO—which again indicates that linear PSO is not suitable for nonlinear models.

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Table VII

<table>
<thead>
<tr>
<th>Scene</th>
<th>ARE Scores</th>
<th>Execution Times</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>BiPSO</td>
<td>Fan-NMF</td>
</tr>
<tr>
<td>Moffett Field</td>
<td>0.0063</td>
<td>0.0130</td>
</tr>
<tr>
<td>time(s)</td>
<td>186.08</td>
<td>101.19</td>
</tr>
<tr>
<td>Indian Pine</td>
<td>0.0115</td>
<td>0.0131</td>
</tr>
<tr>
<td>time(s)</td>
<td>23.722</td>
<td>29.374</td>
</tr>
</tbody>
</table>

*Note: the ARE values of SK-Hype were estimated by employing the FM for reconstruction (we cannot obtain other bilinear parameters by SK-Hype).
proposed algorithm and the linear PSO algorithm identified the remaining regions of this class better than the other algorithms, which indicates that PSO can provide better performance than the traditional algorithms. Regarding the last class, we can see that all the algorithms clearly identified the vegetation region. In summary, except for the second class, the proposed algorithm provided a satisfactory performance. Table VII also reveals that the proposed algorithm and the linear PSO algorithm had lower ARI than other algorithms, but that BiPSO better identifies the first class. Therefore, although BiPSO and linear PSO had similar overall performances, the solutions obtained by BiPSO were better than linear PSO. Regarding execution time, BiPSO, Fan-NMF, and linear PSO required more than twenty seconds, while GBM and CNLS required less time than other algorithms. BiPSO was slightly slower (7%) than linear PSO. The reasons are similar to those discussed earlier for the Moffett Field example.

V. CONCLUSION AND FUTURE WORK

In this paper, we have developed a new algorithm for bilinear spectral unmixing of hyperspectral images using PSO. By combining PSO with MO techniques, the proposed algorithm is capable of simultaneously estimating both endmembers and their corresponding fractional abundances and of handling constrained optimization and high-dimensional issues when providing the solution. The proposed method also suggests that swarm intelligence can provide a relatively easy and flexible way to solve the spectral unmixing problem. Our experimental results, conducted using both synthetic and real hyperspectral data, show that the proposed algorithm provides satisfactory unmixing performances, outperforming other established algorithms for nonlinear spectral unmixing. This shows that although the proposed algorithm does not guarantee the global convergence property, it can still achieve a satisfactory solution in practical applications.

As with any new method, there are some remaining challenges that may become issues over time and will need to be considered in future research which are as follows:

1) the proposed method could be extended to incorporate more complex nonlinear models with additional estimated parameters such as the GBM and PPNMM.

2) Because the computations related to the moving and updating operations of the proposed algorithm are quite simple, they can be easily migrated to parallel computing platforms such as general-purpose graphics processing units (GP-GPUs). In future work, we plan to develop a parallel version of the algorithm to improve its computational speed on specialized hardware architectures such as GPUS;

3) The BiPSO framework can be easily modified into a global search algorithm using strategies such as Random PSO and Multistart PSO [57]. However, doing so may be too time-consuming to be practical. Additional global search strategies and mathematical verification should be considered.

ACKNOWLEDGMENT

The authors would like to thank the Jet Propulsion Laboratory for providing the AVIRIS datasets.

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