

A ROBUST MINIMUM VOLUME ENCLOSING SIMPLEX ALGORITHM FOR HYPERSPPECTRAL UNMIXING

ArulMurugan Ambikapathi[†], Tsung-Han Chan[†], Wing-Kin Ma^{†*} and Chong-Yung Chi[†]

[†]Inst. Commun. Eng., National Tsing Hua Univ.
Hsinchu, Taiwan

E-mail: (tsunghan@mx, cychi@ee).nthu.edu.tw

^{*}Dept. Electronic Eng., Chinese Univ. Hong Kong
Shatin, N.T., Hong Kong

E-mail: wkma@ieee.org

ABSTRACT

Hyperspectral unmixing is a process of extracting hidden spectral signatures (or endmembers) and the corresponding proportions (or abundances) of a scene, from its hyperspectral observations. Motivated by Craig's belief, we recently proposed an alternating linear programming based hyperspectral unmixing algorithm called minimum volume enclosing simplex (MVES) algorithm, which can yield good unmixing performance even for instances of highly mixed data. In this paper, we propose a robust MVES algorithm called RMVES algorithm, which involves probabilistic reformulation of the MVES algorithm, so as to account for the presence of noise in the observations. The problem formulation for RMVES algorithm is manifested as a chance constrained program, which can be suitably implemented using sequential quadratic programming (SQP) solvers in an alternating fashion. Monte Carlo simulations are presented to demonstrate the efficacy of the proposed RMVES algorithm over several existing benchmark hyperspectral unmixing methods, including the original MVES algorithm.

Index Terms— Convex analysis, Hyperspectral unmixing, Minimum-volume enclosing simplex, Chance constrained program, Sequential quadratic programming

1. INTRODUCTION

In recent years, lots of attention have been drawn towards hyperspectral unmixing (HU), which decomposes the hyperspectral observations over multiple bands into a collection of endmember signatures and their corresponding proportions (or abundances) [1–8, 13]. The algorithms for HU can generally be classified into two groups. Algorithms in the first group are based on the conventional pure pixel assumption (pixels in the observations that are fully contributed by a single endmember). This includes N-finder (N-FINDER) [2] and vertex component analysis (VCA) [3]. However, for highly mixed data where pure pixels do not exist, these methods may not perform well. Algorithms in the second group are devised without relying on the pure pixel assumption. This includes minimum volume transform (MVT) [4], joint Bayesian algorithm (JBA) [5], and minimum volume simplex analysis (MVSA) [6]. In the development of effective HU algorithms, a key aspect that has raised concerns recently is how to account for the presence of noise. All the algorithms mentioned above, except for JBA [5], inherently assumes no noise being present in the model. JBA employs a Bayesian estimation framework to accommodate this problem. While the criterion of JBA is optimal statistically *per se*, the complexity required to implement it

is a challenge. Recently, Bioucas [7] has improved his MVSA algorithm by incorporating soft (or hinge) constraints, so that the effects of outlier pixels caused by noise can be mitigated.

Very recently, Chan *et al.* developed an alternating linear programming based HU algorithm called minimum volume enclosing simplex (MVES) algorithm [8] based on Craig's belief that the vertices of a minimum-volume simplex enclosing all the observed pixels should serve as a high-fidelity estimates of the endmember signatures [4]. The MVES algorithm is developed by considering a noise-free linear mixing model, and it shows promising results for highly mixed data.

In this paper, we consider a noisy scenario where the observations are corrupted by zero-mean additive white Gaussian noise. Based on Craig's belief [4], we reformulate the HU problem (with noisy observations) as a robust MVES (RMVES) optimization problem. Since the probability distribution of the noise is assumed to be known, we incorporate the chance constraints in the RMVES problem formulation. Our optimization approach to the new problem formulation is to use a divide-and-conquer strategy: we break the original problem into a multitude of subproblems, where each subproblem is less difficult to handle and computationally easier to manage. More specifically, we solve the subproblems in an alternating fashion, where each subproblem is implemented by sequential quadratic programming (SQP) solvers. Through extensive simulations we show that the RMVES algorithm is more robust to noise with better performance especially for data with lower purity levels.

The notations used in this paper are standard. To mention those, \mathbb{R}^M and $\mathbb{R}^{M \times N}$ represent a set of real $M \times 1$ vectors and $M \times N$ matrices, respectively, \mathbf{I}_N is an $N \times N$ identity matrix, $\mathbf{1}_N$ represents an $N \times 1$ all one vector, and $\mathbf{0}$ is an all-zero vector of proper dimension. The symbol \succeq denotes the componentwise inequality, $\|\cdot\|_2$ represents the Euclidean norm, and $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ corresponds to Gaussian distribution with mean vector $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$.

2. PROBLEM STATEMENT AND ASSUMPTIONS

Suppose that a hyperspectral sensor with M spectral bands measures solar electromagnetic radiation reflecting from N distinct substances. Each pixel vector of the measured hyperspectral image cube can be described by an $M \times N$ linear mixing model [1–4]:

$$\mathbf{y}[n] = \mathbf{x}[n] + \mathbf{w}[n], \quad (1)$$

$$\mathbf{x}[n] = \mathbf{A}\mathbf{s}[n] = \sum_{i=1}^N s_i[n]\mathbf{a}_i, \quad \forall n = 1, \dots, L. \quad (2)$$

Here, $\mathbf{y}[n] = [y_1[n], \dots, y_M[n]]^T$ is the n th noisy observed pixel vector comprising M spectral bands, $\mathbf{x}[n] = [x_1[n], \dots, x_M[n]]^T$ is the noise-free counterpart, $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_N] \in \mathbb{R}^{M \times N}$ denotes

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the endmember signature matrix whose i th column vector \mathbf{a}_i is the i th endmember signature, $\mathbf{s}[n] = [s_1[n], \dots, s_N[n]]^T \in \mathbb{R}^N$ is the n th abundance vector comprising N fractional abundances, $\mathbf{w}[n] = [w_1[n], \dots, w_M[n]]^T$ is the zero-mean white Gaussian noise vector (i.e., $\mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_M)$, where σ^2 is the noise variance) and L is the total number of observed pixel vectors.

The goal of hyperspectral unmixing is to estimate the endmember signature matrix \mathbf{A} and the abundances $\mathbf{s}[1], \dots, \mathbf{s}[L]$ from the noisy observed pixels $\mathbf{y}[1], \dots, \mathbf{y}[L]$, assuming that the number of endmembers N is known *a priori*.

We consider the following general assumptions that are applicable to HU algorithms :

(A1) (Non-negativity condition) $s_i[n] \geq 0 \forall i, n$.

(A2) (Full additivity condition) $\sum_{i=1}^N s_i[n] = 1 \forall n$.

(A3) $\min\{L, M\} \geq N$ and \mathbf{A} is of full column rank.

(A1) and (A2) are valid assumptions in hyperspectral imaging because the abundances are fractional proportions [1–4]. In addition, the number of pixels and that of spectral bands involved are larger than the number of endmembers and each endmember has its unique signature, which justifies (A3).

Before getting into the core of development, we need to describe a basic, essential concept in MVES, namely convex hull and simplex [9]. Given a set of vectors $\{\mathbf{a}_1, \dots, \mathbf{a}_N\} \subset \mathbb{R}^M$, the *convex hull* of $\{\mathbf{a}_1, \dots, \mathbf{a}_N\}$ is defined as

$$\text{conv}\{\mathbf{a}_1, \dots, \mathbf{a}_N\} = \left\{ \mathbf{x} = \sum_{i=1}^N \theta_i \mathbf{a}_i \mid \mathbf{1}_N^T \boldsymbol{\theta} = 1, \boldsymbol{\theta} \succeq \mathbf{0} \right\}, \quad (3)$$

where $\boldsymbol{\theta} = [\theta_1, \dots, \theta_N]^T \in \mathbb{R}^N$. In addition, a convex hull $\text{conv}\{\mathbf{a}_1, \dots, \mathbf{a}_N\}$ is called a *simplex* if $M = N - 1$ and $\mathbf{a}_1, \dots, \mathbf{a}_N$ are affinely independent.

3. REVIEW OF MVES PROBLEM FORMULATION

The noise-free signal model given by (2) is considered here for reviewing the formulation and theory behind MVES problem [8]. Like many other HU algorithms [1], we begin with dimension reduction of the observed pixels by projecting them onto an observed-pixel-constructed affine set [8, 10], as given in the following lemma:

Lemma 1. (Dimension reduction by affine set fitting [8]) Under (A2) and (A3), the dimension-reduced pixel vector $\tilde{\mathbf{x}}[n]$ can be obtained by an affine transformation of $\mathbf{x}[n]$:

$$\tilde{\mathbf{x}}[n] = \mathbf{C}^T (\mathbf{x}[n] - \mathbf{d}) \in \mathbb{R}^{N-1}, \quad (4)$$

where (\mathbf{C}, \mathbf{d}) is the affine set fitting solution given by

$$\mathbf{d} = \frac{1}{L} \sum_{n=1}^L \mathbf{x}[n], \quad (5)$$

$$\mathbf{C} = [\mathbf{q}_1(\mathbf{U}\mathbf{U}^T), \mathbf{q}_2(\mathbf{U}\mathbf{U}^T), \dots, \mathbf{q}_{N-1}(\mathbf{U}\mathbf{U}^T)], \quad (6)$$

where $\mathbf{U} = [\mathbf{x}[1] - \mathbf{d}, \dots, \mathbf{x}[L] - \mathbf{d}] \in \mathbb{R}^{M \times L}$, and $\mathbf{q}_i(\mathbf{R})$ denotes the eigenvector associated with the i th principal eigenvalue of \mathbf{R} .

An important remark related to Lemma 1 is as follows:

(R1) The affine set fitting solution of the noisy observed pixels $(\hat{\mathbf{C}}, \hat{\mathbf{d}})$ (obtained from (5) and (6) by replacing $\mathbf{x}[n]$ with $\mathbf{y}[n]$) gives a best approximation in the least-squares sense [10], and it asymptotically approaches the true (\mathbf{C}, \mathbf{d}) for large L .

Since $\sum_{j=1}^N s_j[n] = 1$ [(A2)], it follows by substituting the noise-free signal model (2) into (4) that

$$\tilde{\mathbf{x}}[n] = \sum_{j=1}^N s_j[n] \boldsymbol{\alpha}_j, \quad (7)$$

where $\boldsymbol{\alpha}_j = \mathbf{C}^T (\mathbf{a}_j - \mathbf{d}) \in \mathbb{R}^{N-1}$ is the j th dimension-reduced endmember signature. Moreover, due to $s_i[n] \geq 0$ [(A1)], it has been proven in [8] that

$$\tilde{\mathbf{x}}[n] \in \text{conv}\{\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_N\} \subset \mathbb{R}^{N-1}, \quad \forall n \quad (8)$$

and $\text{conv}\{\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_N\}$ is a simplex.

Based on Craig's belief [4], the unmixing problem of finding a minimum volume simplex enclosing all the dimension-reduced pixels can now be written as the following optimization problem [8]:

$$\begin{aligned} \min_{\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_N \in \mathbb{R}^{N-1}} \quad & V(\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_N) \\ \text{s.t.} \quad & \tilde{\mathbf{x}}[n] \in \text{conv}\{\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_N\}, \quad \forall n, \end{aligned} \quad (9)$$

where $V(\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_N)$ is the volume of the simplex $\text{conv}\{\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_N\}$ given by [11]

$$V(\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_N) = \frac{|\det(\mathbf{B})|}{(N-1)!} \quad (10)$$

and $\mathbf{B} = [\boldsymbol{\beta}_1 - \boldsymbol{\beta}_N, \dots, \boldsymbol{\beta}_{N-1} - \boldsymbol{\beta}_N] \in \mathbb{R}^{(N-1) \times (N-1)}$. In addition, by (3), we rewrite the constraint of (9) in terms of \mathbf{B} as

$$\tilde{\mathbf{x}}[n] = \boldsymbol{\beta}_N + \mathbf{B}\boldsymbol{\theta}_n, \quad (11)$$

where $\boldsymbol{\theta}_n \succeq \mathbf{0}$ and $\mathbf{1}_{N-1}^T \boldsymbol{\theta}_n \leq 1$. Hence, problem (9) can be equivalently written as

$$\begin{aligned} \min_{\substack{\mathbf{B} \in \mathbb{R}^{(N-1) \times (N-1)} \\ \boldsymbol{\beta}_N, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_L \in \mathbb{R}^{N-1}}} \quad & |\det(\mathbf{B})| \\ \text{s.t.} \quad & \boldsymbol{\theta}_n \succeq \mathbf{0}, \quad \mathbf{1}_{N-1}^T \boldsymbol{\theta}_n \leq 1, \\ & \tilde{\mathbf{x}}[n] = \boldsymbol{\beta}_N + \mathbf{B}\boldsymbol{\theta}_n, \quad \forall n. \end{aligned} \quad (12)$$

By letting $\boldsymbol{\theta}_n = \mathbf{H}\tilde{\mathbf{x}}[n] - \mathbf{g}$ for all n where $\mathbf{H} = \mathbf{B}^{-1}$ and $\mathbf{g} = \mathbf{B}^{-1}\boldsymbol{\beta}_N$, one can eliminate the variables $\boldsymbol{\theta}_n$ for all n in (12) and come up with

$$\begin{aligned} \max_{\substack{\mathbf{H} \in \mathbb{R}^{(N-1) \times (N-1)}, \mathbf{g} \in \mathbb{R}^{N-1}}} \quad & |\det(\mathbf{H})| \\ \text{s.t.} \quad & \mathbf{1}_{N-1}^T (\mathbf{H}\tilde{\mathbf{x}}[n] - \mathbf{g}) \leq 1, \\ & \mathbf{H}\tilde{\mathbf{x}}[n] - \mathbf{g} \succeq \mathbf{0}, \quad \forall n. \end{aligned} \quad (13)$$

Next, we will show how the MVES problem in (13) can be reformulated for the noisy scenario.

4. ROBUST MVES PROBLEM AND ALGORITHM

Let us consider the noisy signal model given by (1). From (1), (4) and (R1), we get

$$\tilde{\mathbf{y}}[n] \triangleq \hat{\mathbf{C}}^T (\mathbf{y}[n] - \hat{\mathbf{d}}) \cong \tilde{\mathbf{x}}[n] + \hat{\mathbf{C}}^T \mathbf{w}[n], \quad (14)$$

where $\hat{\mathbf{C}}^T \mathbf{w}[n]$ is a random vector following $\mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_{N-1})$ (since $\hat{\mathbf{C}}^T$ is a semi-unitary matrix). Following the footsteps of the MVES problem formulation, the robust MVES problem can be expressed by replacing $\tilde{\mathbf{x}}[n]$ by $\tilde{\mathbf{y}}[n] - \hat{\mathbf{C}}^T \mathbf{w}[n]$ in (13):

$$\begin{aligned} \max_{\mathbf{H}, \mathbf{g}} \quad & |\det(\mathbf{H})| \\ \text{s.t.} \quad & \mathbf{1}_{N-1}^T (\mathbf{H}\tilde{\mathbf{y}}[n] - \mathbf{H}\hat{\mathbf{C}}^T \mathbf{w}[n] - \mathbf{g}) \leq 1, \\ & \mathbf{H}\tilde{\mathbf{y}}[n] - \mathbf{H}\hat{\mathbf{C}}^T \mathbf{w}[n] - \mathbf{g} \succeq \mathbf{0}, \quad \forall n, \end{aligned} \quad (15)$$

where $\mathbf{1}_{N-1}^T \mathbf{H}\hat{\mathbf{C}}^T \mathbf{w}[n] \triangleq z[n]$ and $\mathbf{H}\hat{\mathbf{C}}^T \mathbf{w}[n] \triangleq \mathbf{u}[n]$ are a random variable and a random vector with distributions $\mathcal{N}(0, \sigma^2 \mathbf{1}_{N-1}^T \mathbf{H}\mathbf{H}^T \mathbf{1}_{N-1})$ and $\mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{H}\mathbf{H}^T)$, respectively. Since the constraints in (15) involve randomness, they can be manifested as chance constraints so as to mitigate the noise effects in

the observations. The robust MVES (RMVES) problem (or chance constrained problem) becomes

$$\begin{aligned} \max_{\mathbf{H}, \mathbf{g}} \quad & |\det(\mathbf{H})| \\ \text{s.t.} \quad & \Pr(\mathbf{1}_{N-1}^T \mathbf{H} \tilde{\mathbf{y}}[n] - \mathbf{1}_{N-1}^T \mathbf{g} - 1 \leq z[n]) \geq \eta, \\ & \Pr(\mathbf{h}_i^T \tilde{\mathbf{y}}[n] - g_i \geq u_i[n]) \geq \eta, \forall n, i, \end{aligned} \quad (16)$$

where \mathbf{h}_i^T is the i th row vector of \mathbf{H} , g_i is the i th element of \mathbf{g} , $u_i[n] \sim \mathcal{N}(0, \sigma^2 \|\mathbf{h}_i^T\|_2^2)$ is the i th element of $\mathbf{u}[n]$, and $\eta \in [0, 1]$ is a given probability.

The chance constraints in (16) can be further simplified by normalizing the random variables involved and rearranging the constraints. To show this, consider a general chance constraint:

$$\Pr(t \geq \epsilon) \geq \eta, \quad (17)$$

where $\epsilon \sim \mathcal{N}(\mu, \sigma^2)$ and $t \in \mathbb{R}$. By normalizing (17), we get

$$\Pr\left(\frac{t - \mu}{\sigma} \geq \frac{\epsilon - \mu}{\sigma}\right) \geq \eta, \quad (18)$$

where $(\epsilon - \mu)/\sigma$ is a zero-mean unit-variance Gaussian variable. The left-hand side of (18) is the cumulative distribution function of $(\epsilon - \mu)/\sigma$, that is, $\Phi((t - \mu)/\sigma)$ where

$$\Phi(v) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^v e^{-x^2/2} dx. \quad (19)$$

Hence (18) can be expressed as

$$\Phi\left(\frac{t - \mu}{\sigma}\right) \geq \eta, \quad (20)$$

or, equivalently,

$$t \geq \Phi^{-1}(\eta)\sigma + \mu \quad (21)$$

where Φ^{-1} is the inverse of Φ . Applying the above procedure [(17) through (21)] to the constraints of RMVES problem (16), we can have

$$\begin{aligned} \max_{\mathbf{H}, \mathbf{g}} \quad & |\det(\mathbf{H})| \\ \text{s.t.} \quad & \mathbf{1}_{N-1}^T \mathbf{H} \tilde{\mathbf{y}}[n] - \mathbf{1}_{N-1}^T \mathbf{g} - 1 \leq \\ & \sigma \Phi^{-1}(1 - \eta) \sqrt{\mathbf{1}_{N-1}^T \mathbf{H} \mathbf{H}^T \mathbf{1}_{N-1}}, \\ & \sigma \Phi^{-1}(\eta) \|\mathbf{h}_i^T\|_2 \leq \mathbf{h}_i^T \tilde{\mathbf{y}}[n] - g_i, \forall n, i. \end{aligned} \quad (22)$$

The values of η affect the feasible set of (22) (convex or not). When $\eta > 0.5$ (i.e., $\Phi^{-1}(1 - \eta) < 0$ and $\Phi^{-1}(\eta) > 0$), the constraints are second-order cone constraints (convex). If $\eta = 0.5$ (i.e., $\Phi^{-1}(1 - \eta) = 0$ and $\Phi^{-1}(\eta) = 0$), the problem in (22) reduces to the original MVES problem with linear constraints (convex) as in (13). But if $\eta < 0.5$ (i.e., $\Phi^{-1}(1 - \eta) > 0$ and $\Phi^{-1}(\eta) < 0$), the constraints become non-convex in (\mathbf{H}, \mathbf{g}) . Figure 1 illustrates a scatter plot (for $N = 3$) of the dimension reduced noisy observations and the simplex, $\text{conv}\{\alpha_1, \alpha_2, \alpha_3\}$ obtained by RMVES algorithm (to be presented below) for different η . It can be observed that for $\eta < 0.5$ the solution of RMVES problem approaches the true simplex.

While the feasible set of (22) could be convex or non-convex (depending on η), the objective function of (22) is always non-convex. In what follows, we describe our alternating optimization methodology where we try to form subproblems that have less non-convex components. We consider the cofactor expansion for $\det(\mathbf{H})$ along the i th row:

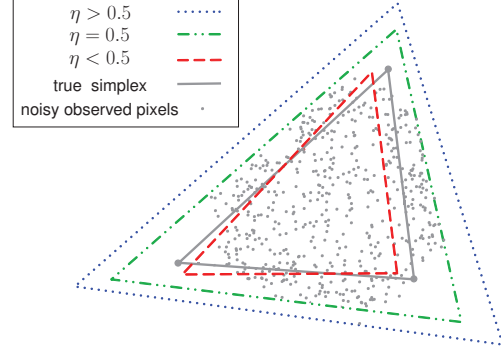


Fig. 1. Scatter plot of the dimension-reduced pixels for $N = 3$, illustrating the solutions of RMVES for different values of η .

$$\det(\mathbf{H}) = \sum_{j=1}^{N-1} (-1)^{i+j} h_{ij} \det(\mathcal{H}_{ij}), \quad (23)$$

where \mathcal{H}_{ij} is the submatrix with the i th row and j th column removed. One can observe from (23) that $\det(\mathbf{H})$ is linear in each \mathbf{h}_i^T , which enables us to update \mathbf{h}_i^T and g_i while fixing the other rows of \mathbf{H} and the other entries of \mathbf{g} . By letting $\mathbf{k}^T = \mathbf{1}_{N-1}^T \mathbf{H}$, the partial maximization of (22) with respect to \mathbf{h}_i^T and g_i can be formulated as

$$\begin{aligned} \max_{\mathbf{h}_i^T, g_i, \mathbf{k}^T} \quad & \left| \sum_{j=1}^{N-1} (-1)^{i+j} h_{ij} \det(\mathcal{H}_{ij}) \right| \\ \text{s.t.} \quad & \mathbf{k}^T = \mathbf{h}_i^T + \sum_{j \neq i} \mathbf{h}_j^T, \\ & \mathbf{k}^T \tilde{\mathbf{y}}[n] - \mathbf{1}_{N-1}^T \mathbf{g} - 1 \leq \sigma \Phi^{-1}(1 - \eta) \|\mathbf{k}^T\|_2, \\ & \sigma \Phi^{-1}(\eta) \|\mathbf{h}_i^T\|_2 \leq \mathbf{h}_i^T \tilde{\mathbf{y}}[n] - g_i, \forall n. \end{aligned} \quad (24)$$

The above problem can be handled by breaking it into two optimization problems, using the same approach as in our predecessor work [8]. Essentially, one is to maximize the term inside the absolute operator of the objective function in (24) with the same constraints, while the other is to minimize it. The two decomposed problems are second-order cone programs if $\eta > 0.5$, linear programs if $\eta = 0.5$ and non-convex problems if $\eta < 0.5$. The optimal solution of (24), denoted by $((\mathbf{h}_i^T)^*, g_i^*)$, is chosen as the optimal solution of the maximization problem if $|p^*| > |q^*|$, and that of the minimization problem if $|q^*| > |p^*|$, where p^* and q^* are the optimal values of the maximization and minimization problems, respectively. This row-wise maximization is conducted cyclically (i.e., $i := (i \text{ modulo } (N - 1)) + 1$ for each row update of \mathbf{H}) until some stopping rule is satisfied.

Suppose that a solution $(\mathbf{H}^*, \mathbf{g}^*)$ is obtained by the above mentioned cyclic maximization. As presented in [8], the endmember signatures can then be recovered by $\hat{\mathbf{a}}_i = \mathbf{C} \hat{\alpha}_i + \mathbf{d}$ for $i = 1, \dots, N$, where

$$\hat{\alpha}_N = (\mathbf{H}^*)^{-1} \mathbf{g}^*, \quad (25)$$

$$[\hat{\alpha}_1, \dots, \hat{\alpha}_{N-1}] = \hat{\alpha}_N \mathbf{1}_{N-1}^T + (\mathbf{H}^*)^{-1}, \quad (26)$$

and the abundance vectors can be estimated as [8]

$$\begin{aligned} \hat{\mathbf{s}}[n] &= [\mathbf{s}'[n]^T \quad 1 - \mathbf{1}_{N-1}^T \mathbf{s}'[n]]^T, \\ &= [(\mathbf{H}^* \tilde{\mathbf{y}}[n] - \mathbf{g}^*)^T \quad 1 - \mathbf{1}_{N-1}^T (\mathbf{H}^* \tilde{\mathbf{y}}[n] - \mathbf{g}^*)^T]^T \end{aligned} \quad (27)$$

Table 1. Average ϕ_{en} and ϕ_{ab} (degrees) over the various unmixing methods for different purity levels (ρ) and SNRs.

Methods	ρ	ϕ_{en}					ϕ_{ab}				
		SNR (dB)					SNR (dB)				
		20	25	30	35	40	20	25	30	35	40
N-FINDR-FCLS	0.7	5.45	5.31	5.24	5.11	5.16	22.54	21.86	21.63	19.76	19.82
	0.85	2.65	2.67	2.66	2.65	2.61	9.60	8.37	8.03	7.93	7.77
	1	1.15	0.58	0.33	0.18	0.10	6.14	3.59	2.13	1.24	0.72
MVSA	0.7	5.95	4.03	2.67	2.12	1.40	20.80	14.56	7.88	4.81	3.14
	0.85	5.99	3.75	2.61	2.07	1.27	19.65	12.12	7.17	4.16	2.34
	1	6.12	3.96	2.71	2.14	1.33	18.93	11.55	6.68	3.85	2.15
MVES	0.7	5.17	3.26	2.43	1.73	1.01	16.66	10.58	6.51	3.81	2.17
	0.85	5.28	3.59	2.65	1.85	1.11	16.88	10.98	7.20	4.26	2.38
	1	6.67	4.37	3.35	2.50	1.55	19.81	13.09	9.58	6.81	4.50
RMVES	0.7	1.69	1.09	0.76	0.46	0.43	9.21	5.37	3.21	1.98	1.32
	0.85	1.90	1.30	1.01	0.53	0.44	8.34	5.90	3.48	2.03	1.38
	1	2.89	2.27	2.05	1.69	1.40	9.75	6.27	5.31	3.32	2.85

for all $n = 1, \dots, L$. To ensure (A1), the negative values of $\hat{s}[n]$ are made zero. The above procedure is referred to as RMVES algorithm.

The proposed RMVES algorithm uses the well known VCA [3] for the initialization of (24) [6]. The optimization problem in (24) is then solved by sequential quadratic programming (SQP). Moreover, in each iteration of the RMVES algorithm (which involves $N - 1$ row updates of \mathbf{H}), we use the solution of the previous iteration as the initialization for the current iteration.

5. SIMULATIONS AND CONCLUSIONS

In this section, the efficacy of the proposed RMVES algorithm is demonstrated using 50 Monte Carlo runs for various purity levels and SNRs. In each run, 1000 noise-free observed pixel vectors were synthetically generated following the signal model in (2), where 6 endmembers (i.e., Alunite, Buddingtonite, Calcite, Copiapite, Kaolinite, and Muscovite) with 417 bands are selected from USGS library [12], and the abundance vectors $\mathbf{s}[n]$ were generated following Dirichlet distribution $D(\mathbf{s}[n], \boldsymbol{\mu})$ with $\boldsymbol{\mu} = \frac{1}{N} \mathbf{1}_N$ [3], for different purity levels $\rho = 0.7, 0.85, 1$ [8]. The noisy data were obtained by adding independent and identically distributed (i.i.d.) zero-mean Gaussian noise to the noise-free data for different SNRs, where $\text{SNR} = \sum_{n=1}^L \|\mathbf{x}[n]\|_2^2 / \sigma^2 ML$. To maintain non-negativity of the noisy observed pixels, we artificially set the negative values of the noisy pixels to zero. For performance comparison, we also tested three existing algorithms, N-FINDR-FCLS [2, 13] (where FCLS [13] was used to find the associated abundances for the endmember estimates of N-FINDR), MVSA [6], and the original MVES [8].

The root-mean-square (rms) spectral angle between the true one and estimated one (which has been widely used in HU [1, 3, 8]) is used as the performance index. We here denote rms spectral angle between endmembers and their estimates as ϕ_{en} , and that between abundance maps and their estimates as ϕ_{ab} . By our extensive numerical experience we found that η (which depends on ρ and SNR) should be less than 0.5 (this can also be justified from Figure 1).

The average ϕ_{en} and ϕ_{ab} of the unmixing algorithms over SNR = 20, 25, ..., 40 dB and $\rho = 0.7, 0.85, 1$ are shown in Table 1, where each bold-faced number denotes the minimum rms spectral angle associated with a specific pair of (ρ , SNR) over all the algorithms. Table 1 shows that the proposed RMVES algorithm yields the best performance for $\rho = 0.7$ and 0.85. For all the values of ρ , the RMVES algorithm is better than its predecessor, the MVES algorithm. In addition, to investigate the problem natures of (22) and (24), we simply performed Monte Carlo simulations by directly solving (22) using SQP for $\rho = 0.7$ and SNR = 20 dB. The average ϕ_{en} and ϕ_{ab} were 9.04 and 24.73 degrees, respectively, which are

apparently much worse than those (1.69 and 9.21) of solving (24) in an alternating fashion (RMVES algorithm). This may be attributed to local optimality issues associated with the highly non-convex nature of (22).

In conclusion, we have presented a robust hyperspectral unmixing method, namely the RMVES algorithm which can effectively unmix the highly mixed and noisy data. The RMVES algorithm applies chance constraints to accommodate the noise effects, and can be suitably implemented using SQP solvers in an alternating fashion. Simulation results showed that the RMVES algorithm outperforms some existing benchmark algorithms and its predecessor MVES algorithm. The application of RMVES algorithm to real hyperspectral data would be our future direction.

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