ON THE ENDMEMBER IDENTIFIABILITY OF CRAIG'S CRITERION FOR HYPERSPECTRAL UNMIXING: A STATISTICAL ANALYSIS FOR THREE-SOURCE CASE

Chia-Hsiang Lin^{*}, ArulMurugan Ambikapathi^{*}, Wei-Chiang Li, and Chong-Yung Chi

Institute of Communications Engineering, National Tsing Hua University, Hsinchu, Taiwan

E-mail: stevenmathmath@gmail.com; aareul@ieee.org; weichiangli@gmail.com; cychi@ee.nthu.edu.tw;

ABSTRACT

Hyperspectral unmixing (HU) is a process to extract the underlying endmember signatures (or simply endmembers) and the corresponding proportions (abundances) from the observed hyperspectral data cloud. The Craig's criterion (minimum volume simplex enclosing the data cloud) and the Winter's criterion (maximum volume simplex inside the data cloud) are widely used for HU. For perfect identifiability of the endmembers, we have recently shown in [1] that the presence of pure pixels (pixels fully contributed by a single endmember) for all endmembers is both necessary and sufficient condition for Winter's criterion, and is a sufficient condition for Craig's criterion. A necessary condition for endmember identifiability (EI) when using Craig's criterion remains unsolved even for three-endmember case. In this work, considering a three-endmember scenario, we endeavor a statistical analysis to identify a necessary and statistically sufficient condition on the purity level (a measure of mixing levels of the endmembers) of the data, so that Craig's criterion can guarantee perfect identification of endmembers. Precisely, we prove that a purity level strictly greater than $1/\sqrt{2}$ is *necessary* for EI, while the same is *sufficient* for EI with probability-1. Since the presence of pure pixels is a very strong requirement which is seldom true in practice, the results of this analysis foster the practical applicability of Craig's criterion over Winter's criterion, to real-world problems.

Index Terms— Hyperspectral unmixing, minimum volume enclosing simplex, purity level, endmember identifiability, statistical analysis

1. INTRODUCTION

Hyperspectral unmixing (HU) is a powerful multidimensional image analysis tool to dissect and characterize the endmember signatures (reflection coefficients of a material) and their corresponding abundances (fractional distributions of a material), from the measured hyperspectral data [2]. The applications of HU include space object identification, military surveillance, retinal analysis, etc., [3]. Based on the seminal works of Craig [4] and Winter [5], a number of powerful HU algorithms have been proposed, and they are recently summarized in [6]. The Craig's criterion in [4] (and the Winter's criterion in [5]) claims that the vertices of the minimum volume simplex enclosing the hyperspectral data cloud (the vertices of the maximum volume simplex inside the data cloud) will yield high fidelity estimates of the endmembers. The Craig's criterion and the Winter's criterion were theoretically analyzed recently in [1], where the necessary and sufficient condition for endmember identifiability (EI) (which is the ability to yield the true endmembers) using Winter's criterion is shown to be the existence of pure pixels (pixels that are completely contributed by a single endmember) for all endmembers. In reality, the presence of pure pixels for all the endmembers is seldom true and hence draws a limit on the practical applicability of Winter's criterion.

In [1], it has also been proved that the existence of pure pixels for all the endmembers is a sufficient condition for EI of Craig's criterion. But, intuitively, geometrically, and by simulations, it can be verified that Craig's criterion can yield perfect identifiability even when the sources are (relatively) highly mixed [7]. However, theoretical analysis of the condition on the mixing level of the sources (i.e., purity levels) for the Craig's criterion to yield the endmember is complicated and remains unsolved for about two decades. In this work, considering a three-source case, we statistically analyze the conditions on the data purity level for which the Craig's criterion can uniquely identify the true endmembers. We begin by studying the relationship between the observations and their corresponding abundances. Then, under a statistical framework, by exploiting the convex geometry of the abundances and by analyzing the property of the minimum volume enclosing simplex (MVES), we derive the conditions for EI of Craig's criterion.

Notations: \mathbb{R}^M and \mathbb{Z}_+ represent the set of real $M \times 1$ vectors and nonnegative integers, respectively. The symbol $\|\cdot\|$ represents the Euclidean norm. \mathbf{e}_i is a unit vector with the *i*th entry equal to 1. Convex hull and affine hull [8] of a set of vectors $\mathbf{a}_1, \ldots, \mathbf{a}_N$ is represented as conv $\{\mathbf{a}_1, \ldots, \mathbf{a}_N\}$, and aff $\{\mathbf{a}_1, \ldots, \mathbf{a}_N\}$, respectively. The relative interior and relative boundary of a set \mathcal{A} are denoted as int(\mathcal{A}) and bd(\mathcal{A}), respectively. $\Pr\{\cdot\}$ denotes the probability function.

2. SIGNAL MODEL AND ASSUMPTIONS

For the purpose of analysis, we consider a noise-free signal model. Following a linear mixing model [1]- [6], each pixel vector (or simply pixel, for convenience) in the observed data \mathbf{x}_n can be represented as:

$$\mathbf{x}_n = \mathbf{A}\mathbf{s}_n = \sum_{i=1}^N s_{in}\mathbf{a}_i, \ \forall n = 1, \dots, L,$$
(1)

where $\mathbf{x}_n = [x_{1n}, \ldots, x_{Mn}]^T$ denotes the *n*th observed pixel vector comprising M spectral bands, \mathbf{a}_i is the *i*th endmember signature, $\mathbf{s}_n = [s_{1n}, \ldots, s_{Nn}]^T \in \mathbb{R}^N$ is the *n*th abundance vector comprising N fractional abundances, and L is the total number of observed pixels. Standard assumptions pertaining to the signal model in (1) are (A1) $s_{in} \ge 0, \forall i, n;$ (A2) $\sum_{i=1}^N s_{in} = 1, \forall n;$ (A3) $M \ge N$, and $\mathbf{A} = [\mathbf{a}_1, \ldots, \mathbf{a}_N]$, where \mathbf{a}_i is the *i*th endmember, is of full column rank [1], [2], [6], [7]. Under (A1) and (A2), it can be noted that the observed pixels \mathbf{x}_n are convex combinations of $\mathbf{a}_1, \ldots, \mathbf{a}_N$, with s_{1n}, \ldots, s_{Nn} as the *unique* combining coefficients, for each \mathbf{x}_n . In other words, $\mathbf{x}_n \in \text{conv}\{\mathbf{a}_1, \ldots, \mathbf{a}_N\}, \forall n$,

^{*}Contributed equally. This work was supported in part by National Science Council (R.O.C.) under Grant NSC 99-2221-E-007-003-MY3 and in part by NTHU and Mackay memorial hospital under Grant 100N2742E1.

and by (A3) conv{ $a_1, ..., a_N$ } is a simplex [9] [10]. As there exists a one-to-one relationship between \mathbf{x}_n and \mathbf{s}_n , for all n, the ensuing EI analysis will be based on \mathbf{s}_n . As a first step in this direction of EI, in this work, we will consider N = 3 (in which case the simplex conv{ a_1, a_2, a_3 } is a triangle and its interior) and $L \to \infty$ (note that the number of pixels can be very large in reality [2]). Precisely, our aim is to find the conditions on \mathbf{s}_n , for which the vertices of the minimum volume simplex enclosing \mathbf{x}_n , for all n (Craig's criterion) will exactly be { a_1, a_2, a_3 }. Below, we define some parameters, sets, and their properties (some illustrated in Figure 1), which will be extensively used in the ensuing analysis.

Definitions and Properties:

- Given an observed data x_n, we define its pixel purity index to be ρ_n ≜ ||s_n||, where s_n is the corresponding abundance vector of x_n. ρ_n ∈ [1/√N = 1/√3, 1] and the bounds are due to (A1) and (A2) [7].
- ρ_n indicates the quantitative dominance of an endmember \mathbf{a}_i in the observed data $\mathbf{x}_n = \sum_{i=1}^3 s_{in} \mathbf{a}_i$ [7]. For instance, $\rho_n = 1$ indicates that the pixel is completely dominated by an endmember and $\rho_n = 1/\sqrt{3}$ indicates that the pixel is heavily mixed, as it is equally contributed by all the 3 endmembers.
- Let $\mathcal{T}_e \triangleq \{\mathbf{s} = [s_1, s_2, s_3]^T \in \mathbb{R}^3 | s_i \ge 0, \sum_{i=1}^3 s_i = 1\} = \operatorname{conv}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, where $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \in \mathbb{R}^3$. Note that \mathcal{T}_e is an equilateral triangle.
- For each $\rho \in [1/\sqrt{3}, 1]$, let $\mathcal{R}(\rho) \triangleq \mathcal{T}_e \bigcap \{ \mathbf{s} \in \mathbb{R}^3 | \|\mathbf{s}\| \le \rho \}$. Then, $\mathcal{R}(\rho_1) \subseteq \mathcal{R}(\rho_2), \forall 1/\sqrt{3} \le \rho_1 \le \rho_2 \le 1$.
- Let $C(\rho) \triangleq \operatorname{aff}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} \bigcap \{\mathbf{s} \in \mathbb{R}^3 | \|\mathbf{s}\| \le \rho\}$, which is a nonempty disc when $\rho \in [1/\sqrt{3}, 1]$, and let $r(\rho)$ be its radius. It is obvious that $C(\rho_1) \subseteq C(\rho_2), \forall 1/\sqrt{3} \le \rho_1 \le \rho_2 \le 1$.
- As $\mathcal{T}_e \subseteq \operatorname{aff}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, note that $\mathcal{R}(\rho) = \mathcal{T}_e \bigcap \mathcal{C}(\rho)$. Also $\mathcal{R}(1) = \mathcal{T}_e$ and $\mathcal{R}(\rho) = \mathcal{C}(\rho)$, $\forall \rho \in [1/\sqrt{3}, 1/\sqrt{2}]$.
- For each simplex *T* in aff {a₁, a₂, a₃} or aff {e₁, e₂, e₃}, we define vol(*T*) to be the Lebesgue measure of *T* with respect to its affine hull [11]. In our case of N = 3, vol(*T*) is just the area of *T*.
- Note that C(1/\sqrt{2}) is exactly the inner tangent circle of the equilateral triangle \$\mathcal{T}_e\$, and thus [12]

$$\operatorname{vol}(\mathcal{T}_e) = 3\sqrt{3}r^2(1/\sqrt{2}).$$
 (2)



Fig. 1. Figure illustrating some notations used in the sequel.

• Let $\mathcal{T}_a \triangleq \operatorname{conv}\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} \subseteq \mathbb{R}^M$ be the simplex that has vertices $\mathbf{a}_1, \mathbf{a}_2$, and \mathbf{a}_3 . Also by (A1) and (A2), $\mathbf{x}_n \in \mathcal{T}_a$ and $\mathbf{s}_n \in \mathcal{T}_e$, for all n.

- We can define a one-to-one transformation T : ℝ³ → ℝ^M, to be the unique linear transformation such that T(e_i) = a_i for i = 1, 2, 3. Clearly, T(v) = Av for each v ∈ ℝ³. Therefore, each vector in T_e can be uniquely mapped to a vector in T_a, and vice versa.
- Since T is linear and it maps the aff{e₁, e₂, e₃} onto the aff{a₁, a₂, a₃}, due to (A3), there exists a positive number α > 0 such that

$$\operatorname{vol}(T(\mathcal{T}_g)) = \alpha \cdot \operatorname{vol}(\mathcal{T}_g), \ \forall \ \mathcal{T}_g \subseteq \operatorname{aff}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\},$$
(3)

$$\operatorname{vol}(T^{-1}(\mathcal{T}_h)) = \alpha^{-1} \cdot \operatorname{vol}(\mathcal{T}_h), \forall \mathcal{T}_h \subseteq \operatorname{aff}\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}, \quad (4)$$

where \mathcal{T}_g and \mathcal{T}_h are simplexes. To determine the constant α , we note that $\operatorname{vol}(\mathcal{T}_a) = \operatorname{vol}(\operatorname{conv}\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}) = \operatorname{vol}(T(\operatorname{conv}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\})) = \alpha \cdot \operatorname{vol}(\operatorname{conv}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\})$, and thus $\alpha = \operatorname{vol}(\mathcal{T}_a)/\operatorname{vol}(\mathcal{T}_e)$.

- For each bounded subset U in aff{a1, a2, a3} or aff{e1, e2, e3}, let MVES(U) be the collection of all the minimum volume enclosing simplexes (triangles for N = 3) that contain U.
- For a given set U ⊆ R³, the conv(U) is defined as the intersection of all the convex sets which contain U [13].
- Let X_L ≜ {x₁,..., x_L} denotes a data set, and define the abundance set of X_L to be S_L ≜ {s₁,..., s_L} where s_n is the corresponding abundance vector of x_n.

Now we can proceed to define a very important concept called purity level.

Definition 1 (Purity Level) A data set \mathcal{X}_L is said to have purity level $\rho \in [1/\sqrt{3}, 1]$, if each vector in its corresponding abundance set \mathcal{S}_L is independently generated with a probability density function (pdf) $f : \mathcal{R}(\rho) \to [0, \infty)$ that satisfies

(A4)
$$\int_{\mathbf{s}\in\mathcal{D}} f(\mathbf{s})d\mathbf{s} > 0, \ \forall \mathcal{D}\subseteq \mathcal{R}(\rho) \ with \ \mathrm{vol}(\mathcal{D}) > 0.$$
 (5)

More generally, for a set, $\lim_{L\to\infty} \mathcal{X}_L$, with purity level ρ , it can be shown that

$$\Pr\{\sup\{\lim_{L \to \infty} \{\rho_1, \dots, \rho_L\}\} = \rho\} = 1,$$
 (6)

where $\sup\{\cdot\}$ denotes supremum of a set and ρ_n is the pixel purity index of $\mathbf{x}_n \in \mathcal{X}_L$. Also note that the pdf in (5) is also very general and *any* meaningful pdf for \mathbf{s}_n will satisfy (5). For instance, the Dirichlet distribution considered in [14] (for \mathbf{s}_n) satisfies this property. The following well-know property [12] will be handy in the EI analysis presented in Section 3:

Property 1 If C is a disc with radius r, then $\mathsf{MVES}(\mathcal{C})$ is exactly the collection of all equilateral triangles with $\mathsf{bd}(\mathcal{C})$ as its inner tangent circle, and they have volume $3\sqrt{3}r^2$. Conversely, if a triangle $\mathcal{T} \supset \mathcal{C}$ and $\operatorname{vol}(\mathcal{T}) = 3\sqrt{3}r^2$, then \mathcal{T} must be an equilateral triangle.

3. ENDMEMBER IDENTIFIABILITY OF MVES

In this section, we will derive the conditions for perfect EI of the Craig's criterion under the premises of (A1) to (A4). The main results are given in the following theorem:

Theorem 1 Assume that the data set \mathcal{X}_L has purity level $\rho \in [1/\sqrt{3}, 1]$, for any $L \in \mathbb{Z}_+$, and $\rho^* \triangleq 1/\sqrt{2}$. Then the following statements are true for endmember identifiability of Craig's criterion:

(S1): If $\mathsf{MVES}(\mathcal{X}_L) = \{\mathcal{T}_a\}$, then $\rho > \rho^*$. (S2): If $\rho > \rho^*$, then $\Pr\{\mathsf{MVES}(\mathcal{X}) = \{\mathcal{T}_a\}\} = 1$, where $\mathcal{X} \triangleq \lim_{L \to \infty} \mathcal{X}_L$.

Proof: We begin to prove Theorem 1 by first observing the *mutual uniqueness* of T_a and T_e , as stated and proved in the following Lemma:

Lemma 1 (Mutual Uniqueness Property)

(L1): $\mathsf{MVES}(\mathcal{X}_L) = \{\mathcal{T}_a\}$ if and only if $\mathsf{MVES}(\mathcal{S}_L) = \{\mathcal{T}_e\}$, (L2): $\mathsf{MVES}(\mathcal{X}) = \{\mathcal{T}_a\}$ if and only if $\mathsf{MVES}(\mathcal{S}) = \{\mathcal{T}_e\}$, where $\mathcal{S} \triangleq \lim_{L \to \infty} \mathcal{S}_L$.

The proof of Lemma 1 is presented in Appendix 4.1. Due to the mutual uniqueness of the MVES of \mathcal{X}_L and \mathcal{S}_L , by considering \mathcal{S}_L we can prove (S1) by contradiction, as follows:

Suppose that $1/\sqrt{3} \le \rho \le 1/\sqrt{2}$. Then, according to (A4), we have $S_L \subseteq \mathcal{R}(\rho) = \mathcal{C}(\rho)$, which implies

$$\operatorname{vol}(\mathcal{U}) \leq \operatorname{vol}(\mathcal{V}), \forall \mathcal{U} \in \mathsf{MVES}(\mathcal{S}_L), \ \forall \mathcal{V} \in \mathsf{MVES}(\mathcal{R}(\rho)).$$
 (7)

Furthermore, since $\mathcal{R}(\rho) = \mathcal{C}(\rho)$ is a disc with radius $r(\rho)$ when $1/\sqrt{3} \le \rho \le 1/\sqrt{2}$, we have from Property 1 that $\mathsf{MVES}(\mathcal{R}(\rho))$ is the collection of all equilateral triangles with $\mathsf{bd}(\mathcal{R}(\rho))$ as inner tangent circle. As a result (from (2)),

$$\operatorname{vol}(\mathcal{V}) = 3\sqrt{3}r^2(\rho) \le \operatorname{vol}(\mathcal{T}_e), \forall \mathcal{V} \in \mathsf{MVES}(\mathcal{R}(\rho)).$$
 (8)

By (7) and (8), $\operatorname{vol}(\mathcal{U}) \leq \operatorname{vol}(\mathcal{T}_e)$ for all $\mathcal{U} \in \mathsf{MVES}(\mathcal{S}_L)$. Obviously when the strict inequality holds, $\mathcal{T}_e \notin \mathsf{MVES}(\mathcal{S}_L)$. On the other hand, when the inequality holds with equality, all the elements in $\mathsf{MVES}(\mathcal{R}(\rho))$, which are infinitely many, are MVES of \mathcal{S}_L , so $\mathsf{MVES}(\mathcal{S}_L) \neq \{\mathcal{T}_e\}$, which, along with (L1) of Lemma 1, completes the proof of (S1) in Theorem 1.

The proof of (S2) of Theorem 1 involves the randomness of S_L . In view of this, we are motivated to study the EI in asymptotic sense. The key result for this proof is stated and proved in the following lemma.

Lemma 2 Suppose that
$$\mathcal{X}_L$$
 has purity level $\rho \in [1/\sqrt{3}, 1]$. Then,
 $\Pr \{ \mathsf{int}(\mathcal{R}(\rho)) \subseteq \mathsf{conv}(\mathcal{S}) \subseteq \mathcal{R}(\rho) \} = 1.$ (9)

The proof of Lemma 2 is presented in Appendix 4.2. As it is obvious that $MVES(\mathcal{R}(\rho)) = MVES(int(\mathcal{R}(\rho)))$ and $MVES(conv(\mathcal{S})) = MVES(\mathcal{S})$, then from Lemma 2 we have

$$\Pr\left\{\mathsf{MVES}(\mathcal{S}) = \mathsf{MVES}(\mathcal{R}(\rho))\right\} = 1.$$
(10)

The above result in (10), relates the EI by the MVES of S to that by the MVES of $\mathcal{R}(\rho)$, where the latter is deterministic and hence more tractable. Indeed, we can identify the necessary and sufficient condition on the purity level ρ for the EI by the MVES of $\mathcal{R}(\rho)$ as described in Lemma 3 below.

Lemma 3 MVES
$$(\mathcal{R}(\rho)) = \{\mathcal{T}_e\}$$
 if and only if $\rho \in (1/\sqrt{2}, 1]$.

The proof of Lemma 3 is presented in Appendix 4.3. Combining (10) and Lemma 3, we can obtain

$$\Pr\left\{\mathsf{MVES}(\mathcal{S}) = \{\mathcal{T}_e\}\right\} = 1,$$

which together with (L2) of Lemma 1 directly yields (S2) of Theorem 1 and thereby completes the proof of Theorem 1.

4. APPENDIX

4.1. Proof of Lemma 1:

(L1): (*Necessity*) We will prove by contradiction. Assume $\mathsf{MVES}(\mathcal{S}_L) \neq \{\mathcal{T}_e\}$, then there exists a simplex $\mathcal{T}'_e \subseteq \mathsf{aff}\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ such that

$$\mathcal{S}_L \subseteq \mathcal{T}'_e, \tag{11}$$

$$\mathcal{T}'_e \neq \mathcal{T}_e,$$
 (12)

$$\operatorname{vol}(\mathcal{T}'_e) \le \operatorname{vol}(\mathcal{T}_e).$$
 (13)

Then we have from (12) and the fact that the linear transformation T is one-to-one, that $T(\mathcal{T}'_e) \neq T(\mathcal{T}_e) = \mathcal{T}_a$. But $T(\mathcal{T}'_e) \subseteq$ aff $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ also satisfies

$$\mathcal{X}_L = \mathbf{A}\mathcal{S}_L = T(\mathcal{S}_L) \subseteq T(\mathcal{T}'_e), \tag{14}$$

$$\operatorname{vol}(T(\mathcal{T}'_{e})) = \alpha \cdot \operatorname{vol}(\mathcal{T}'_{e})$$
$$= (\operatorname{vol}(\mathcal{T}_{a})/\operatorname{vol}(\mathcal{T}_{e})) \cdot \operatorname{vol}(\mathcal{T}'_{e}) \leq \operatorname{vol}(\mathcal{T}_{a}),$$
(15)

where (14) is due to (11), and (15) is due to (3) and (13). Therefore, there exists a simplex $T(\mathcal{T}'_e) \neq \mathcal{T}_a$ that encloses \mathcal{X}_L (by (14)) and has volume not greater than \mathcal{T}_a (by (15)), which implies that $\mathsf{MVES}(\mathcal{X}_L) \neq \{\mathcal{T}_a\}$. Thus the necessity of (L1) is proved.

(*Sufficiency*) This can be proved by following a procedure similar to the above proof of necessity.

(L2): By replacing \mathcal{X}_L , \mathcal{S}_L in the above proof by \mathcal{X} , \mathcal{S} respectively, both necessity and sufficiency of (L2) can be proved.

4.2. Proof of Lemma 2:

Since $S \subseteq \mathcal{R}(\rho)$ by the definition of purity level, $\operatorname{conv}(S) \subseteq \mathcal{R}(\rho)$ is true due to the convexity of $\mathcal{R}(\rho)$. Therefore, it suffices to show that $\Pr\left\{\operatorname{int}(\mathcal{R}(\rho)) \subseteq \operatorname{conv}(S)\right\} = 1$.

Let $\mathcal{Y} \triangleq \{\mathbf{q} \in \operatorname{int}(\mathcal{R}(\rho)) | \mathbf{q} \in \mathbb{Q}^3\}$ be the collection of all rational points in $\operatorname{int}(\mathcal{R}(\rho))$, where \mathbb{Q}^3 denotes the set of rational 3×1 vectors. Then \mathcal{Y} is *countable* and *dense* in $\operatorname{int}(\mathcal{R}(\rho))$ [11].

Fix $\mathbf{y} \in \mathcal{Y}$. Since $\operatorname{int}(\mathcal{R}(\rho))$ is open and $\mathcal{Y} \subseteq \operatorname{int}(\mathcal{R}(\rho))$, there exists $\varepsilon > 0$ and a square $\Box(\mathbf{y}; \varepsilon)$ with center \mathbf{y} and side length ε such that $\Box(\mathbf{y}; \varepsilon) \subseteq \operatorname{int}(\mathcal{R}(\rho))$ [15] (see Figure 2).



Fig. 2. A square $\Box(\mathbf{y}; \varepsilon)$ with center $\mathbf{y} \in \mathcal{Y}$ and side length ε , and its partition

Now we evenly divide $\Box(\mathbf{y}; \varepsilon)$ into 9 sub-squares with side length $\varepsilon' = \varepsilon/3$, and label them by $\Box_1, ..., \Box_9$ (see Figure 2). Since $\operatorname{vol}(\Box_i) = (\varepsilon')^2 = \varepsilon^2/9 > 0$, we have from (A4) that $p \triangleq \int_{\mathbf{s}\in\Box_i} f(\mathbf{s})d\mathbf{s} \in (0, 1]$, and therefore $\Pr\{S \cap \Box_i = \emptyset\} = \lim_{L\to\infty} (1-p)^L = 0$ for each i = 1, ..., 8. Then we have $1 \ge \Pr\{\mathcal{S} \bigcap \Box_i \neq \emptyset \text{ for all } i \in \{1, ..., 8\}\} = 1 - \Pr\{\mathcal{S} \bigcap \Box_i = \emptyset \text{ for some } i \in \{1, ..., 8\}\} \ge 1 - \sum_{i=1}^8 \Pr\{\mathcal{S} \bigcap \Box_i = \emptyset\} = 1 - \sum_{i=1}^8 0 = 1, \text{ that is}$

$$\Pr\{\mathcal{S} \bigcap \Box_i \neq \emptyset \text{ for all } i \in \{1, ..., 8\}\} = 1.$$
 (16) -

Now we define two events E1 and E2, and show that E1 implies E2.

E1:
$$\mathcal{S} \cap \square_i \neq \emptyset$$
 for all $i \in \{1, ..., 8\},$ (17)

E2:
$$\mathbf{y} \in \operatorname{conv}(\mathcal{S}).$$
 (18)

Assume that E1 is true. Then there exists eight vectors $\mathbf{s}_1^{\mathbf{y}}, ..., \mathbf{s}_{\mathbf{y}}^{\mathbf{y}} \in \mathcal{S}$ such that $\mathbf{s}_i^{\mathbf{y}} \in \Box_i$ for each i = 1, ..., 8. But \Box_9 must be contained in $\operatorname{conv}(\mathbf{s}_1^{\mathbf{y}}, ..., \mathbf{s}_{\mathbf{y}}^{\mathbf{y}})$. Thus, $\mathbf{y} \in \Box_9 \subseteq \operatorname{conv}(\mathbf{s}_1^{\mathbf{y}}, ..., \mathbf{s}_{\mathbf{y}}^{\mathbf{y}}) \subseteq \operatorname{conv}(\mathcal{S})$, i.e., E2 is true. Then we have from (16) that $1 = \Pr{\{\mathsf{E1}\}} \leq \Pr{\{\mathsf{E2}\}} \leq 1$, i.e.,

$$\Pr\{\mathbf{y} \in \mathsf{conv}(\mathcal{S})\} = 1 \text{ for each } \mathbf{y} \in \mathcal{Y}.$$
(19)

But \mathcal{Y} can be represented as $\{\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, ...\}$ since it is countable. Thus we have $1 \geq \Pr{\mathcal{Y} \subseteq \mathsf{conv}(\mathcal{S})} = 1 - \Pr{\{\mathbf{y}_i \notin \mathsf{conv}(\mathcal{S})\}} = 1 - \Pr{\{\mathbf{y}_i \notin \mathsf{conv}(\mathcal{S})\}} \geq 1 - \sum_{i=1}^{\infty} \Pr{\{\mathbf{y}_i \notin \mathsf{conv}(\mathcal{S})\}} = 1 - \sum_{i=1}^{\infty} 0 = 1 \text{ (by (19)), that is } \Pr{\mathcal{Y} \subseteq \mathsf{conv}(\mathcal{S})} = 1.$ However, this implies

$$\Pr\{\operatorname{conv}\{\mathcal{Y}\}\subseteq\operatorname{conv}(\mathcal{S})\}=1.$$
(20)

To show $\operatorname{int}(\mathcal{R}(\rho)) \subseteq \operatorname{conv}\{\mathcal{Y}\}$, we fix $\mathbf{z} \in \operatorname{int}(\mathcal{R}(\rho))$ and then prove that $\mathbf{z} \in \operatorname{conv}\{\mathcal{Y}\}$. Since $\operatorname{int}(\mathcal{R}(\rho))$ is open, there exists $\varepsilon'' > 0$ and a square $\Box(\mathbf{z}; \varepsilon'')$ with center \mathbf{z} and side length ε'' such that $\Box(\mathbf{z}; \varepsilon'') \subseteq \operatorname{int}(\mathcal{R}(\rho))$. As before, we evenly divide $\Box(\mathbf{z}; \varepsilon'')$ into 9 sub-squares with side length $\varepsilon''' = \varepsilon''/3$, and label them by $\Box_1', \Box_2', ..., \Box_9'$ (in the same order as in Figure 2). Since $\operatorname{vol}(\Box_i') = (\varepsilon''')^2 = (\varepsilon'')^2/9 > 0$ and \mathcal{Y} is *dense* in $\operatorname{int}(\mathcal{R}(\rho))$, there exist eight vectors $\mathbf{s}_1^{\mathbf{z}}, ..., \mathbf{s}_8^{\mathbf{z}} \in \mathcal{Y}$ such that $\mathbf{s}_i^{\mathbf{z}} \in \Box_i$ for each i = 1, 2, ..., 8. Clearly, \Box_9 must be contained in $\operatorname{conv}\{\mathbf{s}_1^{\mathbf{z}}, ..., \mathbf{s}_8^{\mathbf{z}}\}$, so we have $\mathbf{z} \in \Box_9 \subseteq \operatorname{conv}\{\mathbf{s}_1^{\mathbf{z}}, ..., \mathbf{s}_8^{\mathbf{z}}\} \subseteq \operatorname{conv}\{\mathcal{Y}\}$. Thus we have shown that

$$\operatorname{int}(\mathcal{R}(\rho)) \subseteq \operatorname{conv}\{\mathcal{Y}\}.$$
(21)

Therefore, we have from (20) and (21) that $\Pr \{ \mathsf{int}(\mathcal{R}(\rho)) \subseteq \mathsf{conv}(\mathcal{S}) \} = 1.$

4.3. Proof of Lemma 3:

(*Necessity*) We prove the necessity by contradiction. Suppose that $\rho \in [1/\sqrt{3}, 1/\sqrt{2}]$. Then $\mathcal{R}(\rho) = \mathcal{C}(\rho)$, which is a disc on aff($\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$) with radius $r(\rho)$ (see Figure 3). Thus, by Property 1, MVES($\mathcal{R}(\rho)$) is exactly the collection of infinitely many equilateral triangles with bd($\mathcal{C}(\rho)$) as inner tangent circle. Hence, \mathcal{T}_e is not the unique MVES of $\mathcal{R}(\rho)$, i.e., MVES($\mathcal{R}(\rho)$) $\neq \{\mathcal{T}_e\}$.

(Sufficiency) Fix $\rho \in (1/\sqrt{2}, 1]$. Suppose that $\tilde{\rho} \in [1/\sqrt{2}, 1]$. Then we have from definition of $\mathcal{R}(\rho)$ that

$$\mathcal{R}(1/\sqrt{2}) \subseteq \mathcal{R}(\tilde{\rho}) \subseteq \mathcal{R}(1) = \mathcal{T}_e.$$
 (22)

Let $\mathcal{T}_{\tilde{\rho}} \in \mathsf{MVES}(\mathcal{R}(\tilde{\rho}))$, for each $\tilde{\rho} \in [1/\sqrt{2}, 1]$. Then one can infer from (22) that

$$\operatorname{vol}(\mathcal{T}_{1/\sqrt{2}}) \le \operatorname{vol}(\mathcal{T}_{\tilde{\rho}}) \le \operatorname{vol}(\mathcal{T}_{e}).$$
 (23)

Since $\mathcal{R}(1/\sqrt{2})$ is exactly the disc $\mathcal{C}(1/\sqrt{2})$, by Property 1 and by (2), we have $\operatorname{vol}(\mathcal{T}_{1/\sqrt{2}}) = 3\sqrt{3}r^2(1/\sqrt{2}) = \operatorname{vol}(\mathcal{T}_e)$. Hence, the inequalities in (23) hold with equalities, i.e.,

$$\operatorname{vol}(\mathcal{T}_{\tilde{\rho}}) = \operatorname{vol}(\mathcal{T}_e) = 3\sqrt{3}r^2(1/\sqrt{2}), \ \forall \tilde{\rho} \in [1/\sqrt{2}, 1].$$
(24)



Fig. 3. $\mathcal{R}(\rho)$ when $\rho < 1/\sqrt{2}$ (left) and when $\rho > 1/\sqrt{2}$ (right).

On the other hand, let $1/\sqrt{2} \le \rho' \le \rho'' \le 1$, it is straightforward to see that $\mathcal{R}(\rho') \subseteq \mathcal{R}(\rho'') \subseteq \mathcal{T}_{\rho''}$, so $\mathcal{T}_{\rho''} \in \mathsf{MVES}(\mathcal{T}_{\rho''})$, is also an MVES of $\mathcal{R}(\rho')$ (by (24)), which implies

$$\mathsf{MVES}(\mathcal{R}(\rho'')) \subseteq \mathsf{MVES}(\mathcal{R}(\rho')), \text{ for } 1/\sqrt{2} \le \rho' \le \rho'' \le 1.$$

We would like to note that, since $\mathcal{R}(1) = \mathcal{T}_e$, $\mathsf{MVES}(\mathcal{R}(1))$ is exactly the singleton $\{\mathcal{T}_e\}$, and, by (25), we know that $\mathcal{T}_e \in \mathsf{MVES}(\mathcal{R}(\rho))$.

Thus, what remains to be proved in Lemma 3 is to show that $\mathsf{MVES}(\mathcal{R}(\rho))$ is exactly the singleton $\{\mathcal{T}_e\}$. We prove this by contradiction. Suppose that there exists a simplex \mathcal{T}'_e such that $\mathcal{T}'_e \in \mathsf{MVES}(\mathcal{R}(\rho))$ and $\mathcal{T}'_e \neq \mathcal{T}_e$. By (25), \mathcal{T}'_e is also an MVES of $\mathcal{R}(1/\sqrt{2}) = \mathcal{C}(1/\sqrt{2})$, and it must be an equilateral triangle with $\mathsf{bd}(\mathcal{C}(1/\sqrt{2}))$ as inner tangent circle. Let t be an intersection point of \mathcal{T}'_e and $\mathcal{C}(1/\sqrt{2})$, i.e., $\mathbf{t} \in \mathsf{bd}(\mathcal{T}'_e) \cap \mathsf{bd}(\mathcal{C}(1/\sqrt{2}))$. It is obvious that $\mathbf{t} \in \mathsf{bd}(\mathcal{C}(1/\sqrt{2})) \subseteq \mathsf{int}(\mathcal{C}(\rho))$. On the other hand, since $\mathcal{T}'_e \neq \mathcal{T}_e$, the intersection points of \mathcal{T}'_e and $\mathcal{C}(1/\sqrt{2})$ must be different from those of \mathcal{T}_e and $\mathcal{C}(1/\sqrt{2})$. Hence, $\mathbf{t} \notin \mathsf{bd}(\mathcal{C}(1/\sqrt{2})) \cap \mathsf{bd}(\mathcal{T}_e)$, but this together with $\mathbf{t} \in \mathsf{bd}(\mathcal{C}(1/\sqrt{2}))$ gives $\mathbf{t} \in \mathsf{int}(\mathcal{T}_e)$. Thus $\mathbf{t} \in [\mathsf{bd}(\mathcal{T}'_e) \cap \mathsf{int}(\mathcal{C}(\rho))] \cap [\mathsf{int}(\mathcal{C}(\rho)) \cap \mathsf{int}(\mathcal{T}_e)] = [\mathsf{bd}(\mathcal{T}'_e) \cap \mathsf{int}(\mathcal{C}(\rho))] \cap \mathsf{int}(\mathcal{R}(\rho))$. It is obvious that $[\mathsf{bd}(\mathcal{T}'_e) \cap \mathsf{int}(\mathcal{C}(\rho))] \subseteq \mathsf{bd}(\mathcal{T}'_e \cap \mathcal{C}(\rho))$, thus we obtain

$$\mathbf{t} \in \mathsf{bd}(\mathcal{R}'(\rho)) \cap \mathsf{int}(\mathcal{R}(\rho)),\tag{26}$$

where $\mathcal{R}'(\rho) \triangleq \mathcal{T}'_e \cap \mathcal{C}(\rho)$. However, since $\mathcal{T}'_e \in \mathsf{MVES}(\mathcal{R}(\rho))$, we have $\mathcal{R}(\rho) \subseteq \mathcal{T}'_e$, and hence $\mathcal{R}(\rho) \subseteq \mathcal{R}'(\rho)$. Thus we have $\mathsf{bd}(\mathcal{R}'(\rho)) \cap \mathsf{int}(\mathcal{R}(\rho)) = \emptyset$, which contradicts (26). Therefore, $\{\mathcal{T}_e\}$ must be the unique MVES of $\mathcal{R}(\rho)$.

5. CONCLUSION AND FUTURE DIRECTION

Considering a three-endmember case, the EI analysis for the endmember identifiability of MVES, results in a necessary condition and statistically sufficient condition on the purity level, as stated and proved in Theorem 1. The condition in Theorem 1 reveals that unlike Winter's criterion (where presence of pure pixels for all endmembers i.e., $\rho = 1$ is both necessary and sufficient), the condition required for EI of Craig's criterion (MVES) is much more realistic $(1/\sqrt{2} < \rho \le 1)$ as presence of pure pixels is not necessary. This result fosters the practical applicability of Craig's criterion based algorithms for HU. Interestingly, the Craig's MVES concept is not only used in HU, but also widely used in other blind source separation problems such as biomedical image analysis, gene micro array data analysis etc. The identifiability analysis presented in this paper is a first step in this direction and generalizing the above analysis to any N > 3 is currently under investigation.

6. REFERENCES

- T.-H. Chan, W.-K. Ma, A. Ambikapathi and C.-Y. Chi, "A simplex volume maximization framework for hyperspectral endmember extraction," *IEEE Trans. Geosci. Remote Sens.*, vol. 49, no. 11, pp. 4177-4193, Nov. 2011.
- [2] N. Keshava and J. Mustard, "Spectral unmixing," *IEEE Signal Process. Mag.*, vol. 19, no. 1, pp. 44-57, Jan. 2002.
- [3] P. Shippert, "Why use hyperspectral imagery?," *Photogram., Eng., and Remote Sensing*, vol. 70, no. 4, pp. 377-380, Apr. 2004.
- [4] M. D. Craig, "Minimum-volume transforms for remotely sensed data," *IEEE Trans. Geosci. Remote Sens.*, vol. 32, no. 3, pp. 542-552, May 1994.
- [5] M. E. Winter, "N-findr: An algorithm for fast autonomous spectral end-member determination in hyperspectral data," in *Proc. SPIE Conf. Imaging Spectrometry*, Pasadena, CA, Oct. 1999, pp. 266-275.
- [6] J. M. Bioucas-Dias, A. Plaza, N. Dobigeon, M. Parente, P. G. Q. Du, and J. Chanussot, "Hyperspectral unmixing overview: Geometrical, statistical, and sparse regression-based approaches," *IEEE J. of Sel. Topics in Applied Earth Obs. and Remote Sensing*, vol. 5, no. 2, pp. 354-379, June 2012.
- [7] T.-H. Chan, C.-Y. Chi, Y.-M. Huang, and W.-K. Ma, "A convex analysis based minimum-volume enclosing simplex algorithm for hyperspectral unmixing," *IEEE Trans. Signal Processing*, vol. 57, no. 11, pp. 4418-4432, Nov. 2009.
- [8] S. Boyd and L. Vandenberghe, *Convex Optimization*, UK: Cambridge Univ. Press, 2004.
- [9] A. Ambikapathi, T.-H. Chan, C.-Y. Chi, and K.Keizer, "Hyperspectral data geometry based estimation of number of endmembers using pnorm based pure pixel identification," to appear in *IEEE Trans. Geosci. Remote Sens.*, 2012 (currently available at *IEEE Xplore*).
- [10] A. Ambikapathi, T.-H. Chan, W.-K. Ma, and C.-Y. Chi, "Chance constrained robust minimum volume enclosing simplex algorithm for hyperspectral unmixing," *IEEE Trans. Geosci. Remote Sens.*, vol. 49, no. 11, pp. 4194-4209, Nov. 2011.
- [11] R. L. Wheeden and A. Zygmund, Measure and Integral: An Introduction to Real Analysis, Marcel Dekker Inc., New York, 1977.
- [12] B. J. McCartin, Mysteries of the Equilateral Triangle, Hikari Ltd., 2010.
- [13] D. P. Bertsekas, Convex Optimization Theory, Athena Scientific, 2009.
- [14] J. Nascimento and J. Bioucas-Dias, "Hyperspectral unmixing based on mixtures of Dirichlet components," *IEEE Trans. Geosci. Remote Sens.*, vol. 50, no. 3, pp. 863-878, Mar. 2012.
- [15] T. M. Apostol, Mathematical Analysis, 2nd Edition, Pearson Edu. Taiwan Ltd., 2007.