CONVEX SET AND LINEAR MIXING MODEL; P. Xu and R. Greeley, *Department of Geology, Arizona State University, Tempe, Arizona 85287-1404*

Summary. A major goal of optical remote sensing is to determine surface compositions of the Earth and other planetary objects. For assessment of composition, single pixels in multi-spectral images usually record a mixture of the signals from various materials within the corresponding surface area. In this report, we introduce a closed and bounded convex set as a mathematical model for linear mixing. This model has a clear geometric implication because the closed and bounded convex set is a natural generalization of a triangle in n-space. The endmembers are extreme points of the convex set. Every point in the convex closure of the endmembers is a linear mixture of those endmembers, which is exactly how linear mixing is defined. With this model, some general criteria for selecting endmembers could be described. This model can lead to a better understanding of linear mixing models.

Introduction. A major goal of optical remote sensing is to determine surface compositions of the Earth and other planetary objects. In order to quantify the areal abundances of surface materials, the effects of atmospheric attenuation, illumination geometry, and particle size must be removed from the data, as discussed elsewhere [3]. For assessment of composition, single pixels in multi-spectral images usually record a mixture of the signals from various materials within the corresponding surface area. Two types of models are generally used to quantify the abundances of surface materials in single pixel: *linear mixing models* (macroscopic scale or "checkerboard") [1,7,9] and *non-linear mixing models* (microscopic scale or intimate) [2,4,6]. Mathematically, linear mixing models are expressed as sets of linear equations in which the spectral mixture is a linear combination of component (endmember) spectra:

$$\sum_{i=1}^{k} f_i \mathbf{Re}_i = \mathbf{Rm} \text{ such that } 0 \le f_i \le 1 \text{ for all } i \text{ and } \sum_{i=1}^{k} f_i = 1 \qquad (1)$$

in which **Rm** is the column vector of the spectral mixture, $\mathbf{Re}_i$ is the column vector of *ith* endmember spectral, f_i is the fraction of *ith* endmember in the spectral mixture, and k is the number of endmembers. As a first-order approximation, non-linear mixing models can also be expressed as a set of linear equations except that the reflectance (**R**) is replaced by single-scattering albedo (**W**) in equation (1) [4,8]. In this report, we show how models can be related to a convex set for application to both linear and non-linear mixing models (the effects of instrumental noise are not discussed).

Convex Set. The following definitions and theorems regarding convex set are from [5]. Let v_1, v_2, v_3 be different vectors or points in n-space; the *line segment* is the set of all points: $t_1v_1 + t_2v_2$, with $t_1, t_2 \ge 0$ and $t_1 + t_2 = 1$. A *triangle* is the set of points: $t_1v_1 + t_2v_2 + t_3v_3$, $t_i \ge 0$ for i =1,2,3 and $t_1 + t_2 + t_3 = 1$. Let S be a subset of $\mathbf{R}^n$, S is *convex* if given points P, Q in S, the line segment joining P to Q is also contained in S. Let S be a convex set and let P be a point of S, P is an *extreme point* of S if there do not exist points Q_1, Q_2 of S with $Q_1 \neq Q_2$ such that P can be written in the form: $P = tQ_1 + (1-t)Q_2$ with $0 < t < 1$. Some theorems about convex set are:

(1) Let $P_1, ..., P_n$ be points of $\mathbf{R}^m$. Any convex set which contains $P_1, ..., P_n$ also contains all linear combinations $x_1P_1 + ... + x_nP_n$, such that $0 \le x_i \le 1$ for all i, and $x_1 + ... + x_n = 1$.

(2) Let $P_1, ..., P_n$ be points of $\mathbf{R}^m$. The set of all linear combinations $x_1P_1 + ... + x_nP_n$ with $0 \le x_i \le 1$ for all i, and $x_1 + ... + x_n = 1$, is a convex set which is also called the convex closure of points $P_1, ..., P_n$.

(3) Let S be a closed, bounded, convex set. Then S is the convex closure of its extreme points.

Convex Set and Linear Mixing Model. From the definitions and theorems about the convex set, we see a correspondence between the closed, bounded convex set and linear mixing models.

CONVEX SET AND LINEAR MIXING MODEL: Xu, P. and Greeley, R.

We view the spectra of endmembers and their mixture as vectors or points in n-space. Then the endmembers correspond to extreme points of a convex set and the set of all possible mixtures of the endmembers correspond to the convex set which is the convex closure of its extreme points. We propose that closed and bounded convex set be a mathematical model for linear mixing. The advantages of this model are that: (1) the endmember of linear mixing is clearly stated as an extreme point; (2) the closed and bounded convex set is a natural generalization of a triangle in n-space which has geometric implication; and (3) every point in the convex closure of the endmembers satisfies the condition that the fraction of each endmember in the mixture is non-negative and all fractions equal unity. However, in the linear equation representation of linear mixing, the geometric significance is not apparent and the endmembers are not checked for their extremity. In the light of the convex set, the linear mixing model involves the following steps:

(1) define all the possible endmembers which could be selected from either a spectral library or the multi-spectral images;
(2) find at least two endmembers which constitute the smallest convex set which "contain" the mixture point (this "containment" may be in a least-square sense);
(3) solve the linear equations to obtain the fractions of each endmembers in the mixture.

If step (2) fails, it means that the mixture point is not in any of the convex closures of the endmembers defined in step (1) or that the endmembers defined in step (1) cannot model the mixture. Step (2) ensures that the fraction solutions of step (3) are not negative, nor greater than one. With the convex set model, some general criteria for endmember selection can be formulated. When the endmember is selected from multi-spectral images, the extreme point or vertex of the data cluster would generally be a better candidate. The third endmember should not be in the line segment joining the other two endmembers. Generally speaking, an endmember in the convex closure of the other endmembers is not a good choice of endmember. However, there may be the case in which an endmember is in the convex closure of the other endmembers; if so, the endmembers should be broken into several groups and the mixture will have the fractions in terms of only one group of endmembers.

Conclusions. There is correspondence between a closed, bounded convex set and linear mixing models. We propose that the closed and bounded convex set be a mathematical model for linear mixing. This model has a clear geometric implication because the closed and bounded convex set is a natural generalization of a triangle in n-space. The endmembers are extreme points of the convex set. Every point in the convex closure of the endmembers is a linear mixture of those endmembers, which is exactly how linear mixing is defined. With this model, some general criteria for selecting endmembers could be described. This model can lead to a better understanding of linear mixing models.

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