ISPRS Journal of Photogrammetry and Remote Sensing 131 (2017) 147–159

Contents lists available at ScienceDirect

ISPRS Journal of Photogrammetry and Remote Sensing

journal homepage: www.elsevier.com/locate/isprsjprs

Pure endmember extraction using robust kernel archetypoid analysis for hyperspectral imagery

Weiwei Sun [a,b,*], Gang Yang [a], Ke Wu [c], Weiyue Li [d], Dianfa Zhang [a]

[a] Department of Geography and Spatial Information Techniques, Ningbo University, Ningbo, Zhejiang 315211, China
[b] State Key Lab of Information Engineering on Survey, Mapping and Remote Sensing, Wuhan University, Wuhan, Hubei 430079, China
[c] Institute of Geophysics and Geomatics, China University of Geosciences, Wuhan 430074, China
[d] Institute of Urban Studies, Shanghai Normal University, Shanghai 200234, China

A R T I C L E I N F O

Article history:
Received 15 March 2017
Received in revised form 30 June 2017
Accepted 7 August 2017

Keywords:
Endmember extraction
Pure pixels
Robust kernel archetypoid analysis
Hyperspectral imagery
Archetypal analysis

A B S T R A C T

A robust kernel archetypoid analysis (RKADA) method is proposed to extract pure endmembers from hyperspectral imagery (HSI). The RKADA assumes that each pixel is a sparse linear mixture of all endmembers and each endmember corresponds to a real pixel in the image scene. First, it improves the re8gular archetypal analysis with a new binary sparse constraint, and the adoption of the kernel function constructs the principal convex hull in an infinite Hilbert space and enlarges the divergences between pairwise pixels. Second, the RKADA transfers the pure endmember extraction problem into an optimization problem by minimizing residual errors with the Huber loss function. The Huber loss function reduces the effects from big noises and outliers in the convergence procedure of RKADA and enhances the robustness of the optimization function. Third, the random kernel sinks for fast kernel matrix approximation and the two-stage algorithm for optimizing initial pure endmembers are utilized to improve its computational efficiency in realistic implementations of RKADA, respectively. The optimization equation of RKADA is solved by using the block coordinate descend scheme and the desired pure endmembers are finally obtained. Six state-of-the-art pure endmember extraction methods are employed to make comparisons with the RKADA on both synthetic and real Cuprite HSI datasets, including three geometrical algorithms vertex component analysis (VCA), alternative volume maximization (AVMAX) and orthogonal subspace projection (OSP), and three matrix factorization algorithms the preconditioning for successive projection algorithm (PreSPA), hierarchical clustering based on rank-two nonnegative matrix factorization (H2NMF) and self-dictionary multiple measurement vector (SDMMV). Experimental results show that the RKADA outperforms all the six methods in terms of spectral angle distance (SAD) and root-mean-square-error (RMSE). Moreover, the RKADA has short computational times in offline operations and shows significant improvement in identifying pure endmembers for ground objects with smaller spectrum differences. Therefore, the RKADA could be an alternative for pure endmember extraction from hyperspectral images.

1. Introduction

Hyperspectral imaging collects hundreds of narrow bands of ground objects on the earth surface, and it can be used in identifying and recognizing spectrum divergences among different materials (Bioucas-Dias et al., 2013; Tong et al., 2014). The obtained hyperspectral imagery (HSI) has shown great potentials in many realistic applications including ocean monitoring (Wong and Minnett, 2016; Pan et al., 2017), mine exploration (Petit et al., 2017), precision agriculture (Moharana and Dutta, 2016), land cover mapping (Clark and Kilham, 2016) and so on. Unfortunately, relatively low spatial resolutions with respect to high spectral resolutions of imaging spectrometer, together with homogenous mixture of distinct materials, render that the observed spectral signature at each pixel is actually a spectral mixture of several pure materials (i.e., endmembers) (Tang et al., 2014; Sun et al., 2016; Xu et al., 2015; Zhong et al., 2016). Spectral mixture reduces the power of hyperspectral imagers for real applications mentioned above. Therefore, spectral unmixing is urgent to recover spectral signatures of endmembers present in the image scene, and

* Corresponding author at: Department of Geography and Spatial Information Techniques, Ningbo University, Ningbo, Zhejiang 315211, China.
E-mail address: sunweiwei@nbu.edu.cn (W. Sun).

http://dx.doi.org/10.1016/j.isprsjprs.2017.08.001
0924-2716/

meanwhile to quantify the fractions or proportions of each endmember at each mixed pixel (Bioucas-Dias et al., 2012; Ma et al., 2014; Xu and Shi, 2017).

Hyperspectral unmixing includes two main stages, endmember extraction and abundance estimation. Endmember extraction is a preliminary but key work for hyperspectral unmixing, regardless of its linear or nonlinear models supposed (Bioucas-Dias et al., 2012; Tang et al., 2015; Zhang et al., 2017). Proper endmembers can further bring about accurate abundance estimation for each pixel and guarantee good performance of spectral unmixing, and vice versa. Generally, spectral signatures of endmembers can be extracted from two different schemes (Ambikapathi et al., 2011; Liu et al., 2017): (1) the reference-endmembers are manually measured on the ground or in the library using the field spectroradiometer, and (2) the image-endmembers are extracted from hyperspectral images using endmember extraction algorithms. The spectrum of reference-endmembers usually disagrees with those of image pixels because they have different collecting conditions from hyperspectral imaging (e.g., image sensors, atmospheric effects and scattering conditions) (Stagakis et al., 2016; Zhang et al., 2017). Complicated processing in spectral calibrations is mandatorily requiring for spectral matching between reference-endmembers and the image pixels. In contrast, the image-endmembers are directly estimated from the image scene and simpler procedures bring them more popularity in spectral unmixing (Fu et al., 2015; Sun et al., 2016; Xu and Shi, 2017).

Numerous image-endmember extraction methods have been proposed in current literatures, and they utilize two divergent schemes (Bioucas-Dias et al., 2012): (1) non-pure pixel scheme and (2) pure pixel scheme. The non-pure endmember scheme assumes that no pure pixels exist in the image scene and it seeks artificial pure pixels or "virtual" endmembers for the HSI data. Typical methods include minimum volume simplex analysis, convex analysis-based minimum volume enclosing simplex, independent component analysis and Bayesian approaches (Bioucas-Dias et al., 2012; Dobigeon et al., 2014). Pure-pixel scheme regards that at least one pure pixel exists in the image scene and aims to find pure pixels that contain only one material at the pixel. In this study, we focus our work on the pure-pixel scheme and investigate the pure endmember extraction problem for the hyperspectral images.

Researchers have made great achievements in the pure endmember extraction, and relevant methods can be classified into two main aspects: (1) geometrical methods and (2) matrix factorization methods. The benchmark of geometrical method is pixel purity index (PPI) (Chang and Plaza, 2006). It iteratively projects each spectral vectors onto skewers that are defined as a large set of random vectors, and then chooses the extreme pixels with highest accounting scores as the final endmembers. N-FINDER estimates pure endmember signatures that correspond to a set of pixels defining the largest volume by inflating a simplex inside the HSI dataset (Winter, 1999). The alternative volume maximization (AVMAX) was inspired from N-FINDER, and it maximizes the volume of the simplex defined by the endmembers with respect to only one endmember at one time (Chan et al., 2013). The vertex component analysis (VCA) determines endmembers from the extreme of the projection that has the random direction orthogonal to the subspace spanned by the identified endmember signatures at each iteration (Nascimento and Dias, 2005). The successive volume maximization (SVMAX) improves from VCA, and their slight difference is that SVMAX utilizes the complete subspace whereas VCA considers the random direction in the subspace. The simplex growing algorithm (SGA) iteratively grows a simplex by finding the vertices corresponding to the maximum volume (Chang et al., 2006). Unfortunately, the above geometrical methods utilize the random initial conditions and hence suffer from the unreproducibility problem in realistic applications (Chang, 2013). Moreover, these approaches find one endmember after another via iterative procedure, which would bring about high computation when the number of pixels and endmembers in the image scene is significantly large (Ambikapathi et al., 2011).

In recent years, owning to random projections and convex optimization in compressive sensing (Donoho, 2006), many matrix factorization methods have been presented to handle the pure endmember extraction problem (Fu et al., 2015; Gillis and Ma, 2015). These methods formulate a convex equation of matrix factorization with many additive constraints (e.g., sparsity, low rank or positivity) to simultaneously estimate all the pure endmembers (Ma et al., 2014), and they can be grouped into two main aspects: (1) separable nonnegative matrix factorization (Separable-NMF) methods and (2) sparse self-representation methods. The Separable-NMF methods stand on the linear mixture model and pure pixel assumption, and they transfer the pure endmember extraction into the problem of nonnegative matrix factorization under the separability condition (Gillis and Vavasis, 2014). The separability condition purifies the blind estimation of regular NMF and guarantees the existence of pure pixels in the image scene. Representative algorithms include the hierarchical clustering based on rank-two nonnegative matrix factorization (H2NMF) (Gillis et al., 2015) and recursive nonnegative matrix factorization (RNMF) (Gillis and Vavasis, 2014). In contrast, the sparse self-representation methods utilize the self-representation property of the HSI data, and devise the pure endmember extraction into a joint sparse recovery problem by using the HSI dataset itself as a dictionary (Qu et al., 2015). The subspace vertex pursuit (SVP) (Qu et al., 2015) and self-dictionary multiple measurement vector (SDMMV) (Fu et al., 2015) are exampled as their typical algorithms. For example, H2NMF considers the small-sized materials as noise or outliers, which would negatively affect the endmember estimation. (Bioucas-Dias et al., 2012). The SDMMV is only robust to noise perturbations with sufficiently small levels and that definitely degrades its performance in some realistic hyperspectral images with bigger noise (Fu et al., 2015).

In this paper, inspired by archetypal analysis (AA) (Cutler and Breiman, 1994), we propose a robust kernel archetypoid analysis (RKADA) method to investigate the pure endmember extraction problem in the HSI data. Our motivation is to improve the convex equation of AA with a new binary sparse constraint, to promote the robustness of optimization function and its computational speeds, and to apply the proposed method in the field of pure endmember extraction problem on realistic hyperspectral images. A few scholars have made some works on AA for spectral unmixing in HSI data (Sun et al., 2016; Zhao et al., 2015, 2016; Zhao et al., 2017). For example, Zhao introduced AA into spectral unmixing and tested the kernel archetypal analysis (KAA) in multiple endmember extraction for the HSI scenario without pure endmembers (Zhao et al., 2015). After that, he implemented the Nystrom method to accelerate computation speeds of Gaussian kernel matrix and presented a fast version of KAA for endmember extraction and multilayer unmixing on the HSI data (Zhao et al., 2017, 2016). Although the works by Zhao and us adopt similar kernel functions into AA to investigate the spectral unmixing problem of the HSI data, our proposed RKADA method differs from his work in three main aspects. (1) Our method is proposed for extracting pure endmembers whereas previous works by Zhao were concentrated in the scenario of HSI data without pure endmembers. The proposed RKADA originates from the archetypoid analysis (ADA), which is an improved model of AA, and it assumes that the archetypoids or pure endmembers correspond to real pixels in the image scene. In contrast, the KAA by Zhao originates from AA, and it assumes that the archetypes or endmembers are a linear mixture of all the pixels. Their assumptions determine that the extracted endmembers are "virtual" endmembers and do not exist in the image scene. (2) Our