CSIAM Trans. Appl. Math.
doi: 10.4208/csiam-am.SO-2021-0001

Vol. 3, No. 1, pp. 109-132
March 2022

Gradient Type Methods for Linear Hyperspectral Unmixing

Fangfang Xu[1,*], Yating Wang[1], Yanyan Li[1], Lu Liu[2] and Tonghua Tian[3]

[1] *College of Mathematics and Systems Science, Shandong University of Science and Technology, Qingdao 266590, P.R. China.*
[2] *Institute of Software, Chinese Academy of Sciences, Beijing 100190, P.R. China.*
[3] *School of Operations Research and Information Engineering, Cornell University, Ithaca, NY, USA.*

Received 2 January 2021; Accepted 7 July 2021

Abstract. Hyperspectral unmixing (HU) plays an important role in terrain classification, agricultural monitoring, mineral recognition and quantification, and military surveillance. The existing model of the linear HU requires the observed vector to be a linear combination of the vertices. Due to the presence of noise, or any other perturbation source, we relax this linear constraint and penalize it to the objective function. The obtained model is solved by a sequence of gradient type steps which contain a projection onto the simplex constraint. We propose two gradient type algorithms for the linear HU, which can find vertices of the minimum volume simplex containing the observed hyper-spectral vectors. When the number of given pixels is huge, the computational time and complexity are so large that solving HU efficiently is usually challenging. A key observation is that our objective function is a summation of many similar simple functions. Then the computational time and complexity can be reduced by selecting a small portion of data points randomly. Furthermore, a stochastic variance reduction strategy is used. Preliminary numerical results showed that our new algorithms outperformed state-of-the-art algorithms on both synthetic and real data.

AMS subject classifications: 65K05, 68W20, 90C30

Key words: Hyperspectral unmixing, minimum volume simplex, linear mixture model, alternating minimization, proximal gradient method, adaptive moments method, stochastic variance reduction strategy.

1 Introduction

Hyperspectral unmixing (HU) is a source separation problem, which is widely used in terrain classification, agricultural monitoring, mineral recognition and quantification,

*Corresponding author. *Email address:* `xuff@sdust.edu.cn` (F. Xu)

and military surveillance [1, 5, 18, 22]. HU aims at decomposing pixel spectra in a scene into materials, and their corresponding fractional abundances. The materials are also called endmembers, which are generally considered to represent the pure materials present in the image. The set of abundances at each pixel is considered to represent the percentage of each endmember that is occupied in the pixel. The materials in hyperspectral unmixing are statistically dependent and combine in a linear or nonlinear fashion. Because the linear model of hyperspectral unmixing is simple, whose physical meaning is clear, and the solution is satisfactory, it is very suitable for hyperspectral unmixing. We only consider linear hyperspectral unmixing [14, 23, 26, 30] in this paper.

Algorithms of linear hyperspectral unmixing mainly fall into four types: geometrical based approaches [4, 27], statistical based approaches [24, 25], sparse regression based approaches [6], and spatial/spectral joint analysis [29]. The geometrical based approaches can be categorized into two main classes of methods: pure pixel (PP) [27] based and minimum volume (MV) [14] based methods. The pure pixel based algorithms still belong to the minimum volume class but assume the presence in the data of at least one pure pixel per endmember. This kind of algorithm finds the set of the purest pixels in the data, see for instances pixel purity index (PPI) [7, 8], N-FINDR [34], iterative error analysis (IEA) [28], vertex component analysis (VCA) [27], simplex growing (SGA) [12], sequential maximum angle convex cone (SMACC) [16], alternating volume maximization (AVMAX) [11]. The minimum volume approaches seek a mixing matrix M that minimizes the volume of the simplex defined by its columns, referred to as $\mathrm{conv}(M)$, subject to the constraint that $\mathrm{conv}(M)$ contains the observed spectral vectors. The pure pixel constraint is no longer enforced, resulting in a much harder nonconvex optimization problem. The minimum volume approaches include minimum volume simplex analysis (MVSA) [20], simplex identification via variable splitting and augmented Lagrangian (SISAL) [4], minimum volume enclosing simplex (MVES) [10], iterative constrained endmembers (ICE) [3], convex cone analysis (CCA) [17], etc. Geometrical based approaches have a light computational burden and clear conceptual meaning, but may lead to poor results in highly mixed scenarios. Statistical methods are powerful alternative in highly mixed scenarios at the cost of higher computational complexity. They are mainly based on independent component analysis, Bayesian method and non-negative matrix factorization. In sparse regression based unmixing, endmembers are assumed to exist in a huge spectral library, and each pixel of the image can be expressed by the linear combinations of a number of spectra in the spectral library. Because the endmembers are very rare compared to the spectral library, images can be sparsely expressed by the spectral library. Sparse regression based unmixing is an area with strong links to compressed sensing, least angle regression, basis and matching pursuits. Spatial/spectral joint analysis suppose that pixels are not isolated alone, but in a 3D natural scene. The endmembers of the hyperspectral image can be extracted by combining the spectral and spatial information of the surrounding pixels.

The existing model of linear HU requires the observed vector to be a linear combination of the vertices. Due to the presence of noise, or contaminations from other sources,