Spectral Unmixing-Based Clustering of High-Spatial Resolution Hyperspectral Imagery

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Abstract—This paper introduces a novel unsupervised spectral 5 unmixing-based clustering method for high-spatial resolution hy-6 perspectral images (HSIs). In contrast to most clustering methods 7 reported so far, which are applied on the spectral signature repre-8 9 sentations of the image pixels, the idea in the proposed method is to apply clustering on the abundance representations of the pixels. 10 Specifically, the proposed method comprises two main processing 11 stages namely: an unmixing stage (consisting of the endmember 12 extraction and abundance estimation (AE) substages) and a clus-13 tering stage. In the former stage, suitable endmembers are selected 14 first as the most representative pure pixels. Then, the spectral sig-15 nature of each pixel is expressed as a linear combination of the 16 endmembers' spectral signatures and the pixel itself is represented 17 by the relative abundance vector, which is estimated via an efficient 18 AE algorithm. The resulting abundance vectors associated with the 19 20 HSI pixels are next fed to the clustering stage. Eventually, the pixels are grouped into clusters, in terms of their associated abundance 21 22 vectors and not their spectral signatures. Experiments are performed on a synthetic HSI dataset as well as on three airborne 23 24 HSI datasets of high-spatial resolution containing vegetation and 25 urban areas. The experimental results corroborate the effective-26 ness of the proposed method and demonstrate that it outperforms state-of-the-art clustering techniques in terms of overall accuracy, 27 average accuracy, and kappa coefficient. 28

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Index Terms—Abundance estimation (AE), clustering, endmember extraction (EE), hyperspectral imagery (HSI), spectral unmixing (SU).

I. INTRODUCTION

H YPERSPECTRAL imaging has enabled applications and detailed mapping possibilities in a wide variety of Earth studies. In particular, airborne hyperspectral images (*HSIs*) offer high-spatial resolution with detailed spectral accuracy. This versatility enhances the identification, modeling, and detailed classification of various natural and man-made materials. *HSIs* are collected via hyperspectral sensors and are represented as data cubes consisting of numerous contiguous spectral bands of narrow bandwidths. A significant characteristic of *HSIs*, which

Manuscript received September 14, 2016; revised November 21, 2016 and January 24, 2017; accepted March 13, 2017. Manuscript received September 14, 2016. This work was supported by the PHySIS Project under Contract 640174 within the H2020 Framework Program of the European Commission. (*Corresponding author: Eleftheria A. Mylona.*)

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Digital Object Identifier 10.1109/JSTARS.2017.2687703

makes their processing more challenging, is the presence of 42 *mixed pixels*, which depict surface regions consisting of two or 43 more distinct materials. The data for each mixed pixel corre-44 spond to the total reflectance of all the materials present within 45 the pixel in numerous spectral bands from the surface depicted 46 by the pixel, which form the *spectral signature* of the pixel. 47 The key objectives in HSI processing are: 1) the detection of 48 the constituent components of mixed HSI pixels as well as the 49 proportions in which they appear, which will allow the produc-50 tion of abundance maps per material and 2) the identification 51 of spectrally homogeneous regions. The first objective is tack-52 led via spectral unmixing (SU) and the second via the use of 53 clustering algorithms. 54

In this study, we focus on the problem of identifying spec-55 trally homogeneous regions, via clustering (unsupervised) tech-56 niques, which, in contrast to their supervised counterparts, they 57 do not require any externally labeled set of pixels. Most cluster-58 ing techniques proposed in this field are applied on the spectral 59 signature representations of the pixels. In contrast, the key idea 60 of the proposed methodology is to apply clustering on the abun-61 dance vector representations of the HSI pixels, since the latter 62 representation is likely to lead to more well-separated clusters. 63 To this end, SU is applied first on the spectral representations 64 of the pixels, in order to extract the corresponding abundance 65 vectors, and then, clustering is applied on the abundance vector 66 pixels representations. 67

SU [1]-[6] of HSIs has been widely applied to environmental 68 studies. It consists of two main substages, namely 1) endmem-69 ber extraction and 2) abundance estimation (AE). EE [7]-[11] is 70 a challenging process since the aim is to mine the purest pixels 71 (endmembers) of each spectrally distinct material of a HSI. The 72 latter almost always consists of mixed pixels, which are also af-73 fected by noise spectra. Ideally, each endmember ought to have 74 the maximum possible abundance of a single physical material 75 present in the HSI under study and minimum (close to zero) 76 abundance for the rest of the physical materials. Moreover, the 77 determination of the number of endmembers is critical since an 78 underestimated number may result in poor representation of the 79 mixed HSI pixels under study, whereas an overestimated num-80 ber may comprise a lot of mixed signatures. Popular endmember 81 extraction algorithms (EEAs) include VCA [12], N-FINDR vari-82 ants [13], and MVSA [14]. Other related algorithms are discussed 83 in [16]-[18]. 84

The aim of *AE* is the decomposition of the spectral signatures of mixed pixels into a selection of spectral signatures

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corresponding to the reflectance of pure physical materials (end-87 *members*). The latter is usually extracted by the image itself via 88 EE (however, in some cases they are selected from specific 89 90 spectral libraries). AE results in a set of corresponding fractions (abundances), which indicate the proportion of each endmem-91 ber present in a given pixel. Clearly, the ultimate success of AE 92 depends heavily on the appropriate selection of endmembers. 93 Since only a small number of the available materials' spectra 94 are expected to be present in a HSI pixel (especially in high-res-95 96 olution HSIs), the abundance vectors are expected to be sparse. Clustering [19], [20] partitions a set of pixels from the input 97 image into groups. Some of the most known clustering ap-98 proaches are the k-means [21], the Fuzzy C-Means (FCM) [22], 99 the Possibilistic C-Means (PCM) [23] and their variants, e.g., 100 [24], [25]. The aforementioned algorithms are suitable for re-101 covering compact clusters and they use specific vectors, (called 102 representatives) to represent the clusters that underlie in the 103 current dataset. In contrast to these algorithms, that provide a 104 105 single data clustering, in Hierarchical Agglomerative Clustering (HAC) [26], [27], the data are organized into an effective hier-106 107 archy of nested clusterings. HAC requires a metric in order to calculate the dissimilarity between pairs of pixels and a linkage 108 so as to measure the dissimilarity between clusters. 109

110 A. Related Work

It should be mentioned that the literature on clustering tech-111 niques applied on HSIs is limited. In [28], a graph data struc-112 ture is generated to represent the tree crowns weighted with 113 114 the Euclidean distance. A minimum spanning tree is generated using Kruskal's algorithm and edges above a length threshold 115 are removed to generate independent clusters. In [29], an unsu-116 pervised hierarchical cluster analysis to phytoplankton pigment 117 data is applied with the aim of discriminating different phy-118 toplankton assemblages in open ocean environments. Several 119 types of optical data vectors are used as input to HAC including 120 objects consisting of reflectance values of hyperspectral data. 121 Also, in [30], a new clustering algorithm, named Adaptive Pos-122 sibilistic C-Means (APCM), is applied on HSIs. 123

In [31], a clustering procedure is proposed, which consists of 124 three processes: 1) EE, 2) unmixing and 3) hardening process 125 via the winner-takes-all approach, in order to produce recon-126 structed pixels spectra. In [32], the proposed work utilizes the 127 Gauss Mixture Vector Quantization algorithm to learn the mix-128 ture analysis and explores the cluster analysis with correlation 129 distance. In [33], SU is combined with k-means cluster analysis 130 for accurate geological mapping. The data are first classified 131 into two categories: hydrothermal alteration areas and unal-132 tered rocks. SU is applied to hydrothermal alteration areas and 133 134 k-means clustering to unaltered rocks as two separate approaches. In [34], the proposed work generates classification 135 maps based on k-means clustering and Gradient Flow. SU is 136 conducted using the Max-D algorithm to automatically find 137 endmembers. It should be highlighted that, in all previous meth-138 ods, the unmixing and clustering processes are utilized as two 139 separate steps, in the sense that their results are extracted inde-140 141 pendently from each other and are combined next.

In this paper, a novel unsupervised SU-based clustering 142 method (SUBC) for HSIs is proposed. SUBC consists of two 143 processing stages namely: 1) SU, which consists of an EEA, 144 followed by a (sparse) AE algorithm and 2) a clustering algo-145 rithm. The first process identifies suitable endmembers based 146 on the VCA algorithm [12]. Then, AE is applied on each image 147 pixel, in order to provide its abundance representation, using the 148 sparsity-promoting *BiICE* algorithm [35]. Finally, the recently 149 proposed APCM clustering algorithm [30] uses the abundance 150 representations of the pixels, in order to group them into clus-151 ters. It should be noted that the abundance pixel representations 152 adopted in the proposed methodology ensures (in general) a 153 common sparsity pattern for pixels in the same cluster. To the 154 best of our knowledge, this is the first attempt of utilizing the 155 abundance representation of pixels generated by SU as input to 156 a clustering algorithm with the aim to enhance classification in 157 HSIs. 158

The proposed *SUBC* method is evaluated on a synthetic *HSI* 159 dataset as well as on three airborne *HSI* datasets of high-spatial 160 resolution (the agricultural area of Salinas Valley, CA, USA, the 161 land cover at Washington DC Mall, USA, and the urban area of 162 the Pavia center, Italy) and its performance is compared in terms 163 of overall accuracy (*OA*), average accuracy (*AA*) and kappa 164 coefficient with that of state-of-the-art clustering techniques. 165

The paper is organized as follows. Section II introduces the proposed *SUBC* method. Section III demonstrates the results obtained by the proposed method as well as comparisons with state-of-the-art clustering algorithms. Conclusion and future research directions are summarized in Section IV. 170

II. PROPOSED SUBC METHOD

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In this section, we first present the motivation and contribution of this study and then we describe in detail the proposed 173 unmixing-based clustering algorithm. 174

A. Motivation and Contribution

In general, classification algorithms [36], [37] (both super-176 vised and unsupervised) developed so far are applied directly on 177 the *L*-dimensional spectral band vectors of the pixels. However, 178 such (usually high dimensional) representations may contain a 179 lot of redundant information, which may cause pixels depicting 180 different areas to be not well separated from each other in the 181 *L*-dimensional spectral domain. Clearly, this renders the work 182 of the classification algorithms more difficult. Apart from the 183 above issue, most classification schemes used for HSI processing 184 do not focus on exploiting the available fine spectral resolution, 185 that is, they do not consider at all information within the pixel. A 186 further consequence of this is that such schemes do not exploit 187 the fact that each *HSI* pixel contains only a few of the materials 188 existing in the whole HSI (equivalently, the spectral signature of 189 each pixel is expected to result from the linear combination of 190 only a few endmember spectral signatures, which implies that 191 the corresponding abundance vectors will be *sparse*). 192

The approach that we adopt in this paper in order to leverage 193 the above issues is to employ sparsity-promoting SU techniques 194 in order to represent each pixel by its abundance vector (with 195



Fig. 1. Conceptual illustration of the dimensionality reduction achieved, moving from the original band space (usually consisting of hundreds of spectral bands) to the "less correlated" low-dimensional abundance space.

respect to a set of endmembers) and not by its spectral sig-196 197 nature. The rationale behind this choice is twofold. First, the dimension of the abundance vector space (which equals to the 198 199 number of the endmembers depicted in the HSI under study) is usually much lower than the dimension of the spectral signature 200 space (number of spectral bands) (see Fig. 1). Since the cor-201 responding original feature space (the space where each band 202 defines an axis) is high dimensional, the Hughes phenomenon 203 [38] ("curse" of dimensionality) appears. In light of this, the 204 original high-dimensional space of the HSI is transformed to 205 the dimensionally reduced space of abundance vectors [39]. 206

Second, assuming that the endmembers are pure pixels, the 207 (sparse) abundance vectors are expected to form clusters, which 208 209 are likely to lie in different subspaces in the abundance space. It is, thus, anticipated that different classes will form more easily 210 distinguishable clusters in the abundance vectors space. Gener-211 ally speaking, adoption of the abundance representation is ex-212 pected to ease the work of the classification methods. However, 213 214 we have to keep in mind that the abundance retrieval requires a very good estimation of the endmembers that have a physical 215 meaning in order to work properly, which, in practice, is not 216 straightforward. 217

In the SU stage of the SUBC an EEA is first employed, which 218 identifies appropriate endmembers of the image. Next, a sparse 219 220 AE algorithm is used that is based on the endmembers extracted by the EEA, in order to produce the abundance fractions for 221 each pixel, which in turn form the abundance vector of the 222 pixel. These vectors of all pixels are fed to the second stage of 223 the SUBC method, where a clustering algorithm groups pixels 224 225 based on their abundance representations.

An additional feature concerning the mapping to the abun-226 dance space that should be highlighted is that the number of 227 clusters and the number of endmembers are (in general) dif-228 ferent. A cluster formed according to the abundances usually 229 corresponds to a region where a single (or a few) endmembers 230 have high proportion, whereas all other endmembers have low 231 proportions. However, it can also correspond to the mixture of 232 several endmembers of varied proportions. The block diagram 233 of SUBC is depicted in Fig. 2. 234

235 B. Spectral Unmixing

236 1) Endmember Extraction: Aiming at detecting suitable 237 endmembers, we utilize the *VCA* algorithm [12], which takes



Fig. 2. Block diagram of SUBC.

as input the spectral signatures of the pixels, as can be seen in 238 Fig. 2. Each pixel can be viewed as a vector in an L-dimensional 239 Euclidean space, where each spectral band is assigned to one 240 axis of the space. Based on the aforesaid data points, the 241 VCA algorithm returns a prespecified number of endmembers 242 via iteratively projecting data onto a direction orthogonal to 243 the subspace spanned by the endmembers already determined. 244 The new endmember signature corresponds to the extreme 245 of the projection. The algorithm iterates until the number of 246 endmembers is exhausted [12]. Then, SUBC continues in esti-247 mating the abundance fractions of each endmember via AE. 248

2) Abundance Estimation: The selection of appropriate endmembers is crucial so as to correctly estimate the abundance
fractions. Usually, the spectral signature of the pixel, denoted
by *y*, is assumed to follow the Linear Mixing Model [40] according to which it can be expressed as a linear combination of
its endmembers' spectra as follows:

$$y = \Phi x + n \tag{1}$$

where $\Phi = [\varphi_1, \varphi_2, ..., \varphi_p] \in \Re_+^{L \times p}$, $L \gg p$, is the mixing matrix comprising the endmembers' spectra (*L*-dimensional vectors ϕ_i , i = 1, 2, ..., p), \mathbf{x} is a $p \times 1$ vector consisting of the 257 corresponding abundance fractions, named *abundance vector*, 258 and \mathbf{n} is an $L \times 1$ additive noise vector, which is assumed to be 259 a zero-mean Gaussian distributed random vector with independent and identically distributed elements. 261

Due to the physical constraints of the unmixing problem, the 262 abundance fractions for each pixel should satisfy the following 263 two constraints: 264

$$x_i \ge 0, \ i = 1, \ 2, \ ..., \ N, \quad \sum_{i=1}^N x_i = 1$$
 (2)

that is, the abundances should be nonnegative and they must 265 sum to 1. Furthermore, the *abundance* vector is expected to be 266 sparse, i.e., only a few of its elements will be nonzero, since the 267



Fig. 3. (a) Class of the *HSI* containing two subclasses; (b) representation of pixels in the original space; (c) representation of abundance vectors $x = x_1, x_2$; and (d) clustering result emerged from *SUBC*.

area depicted by a single pixel is likely to embed only a small
fraction of the different materials encountered in the whole *HSI*.
In this study, the abundance vector for each pixel is estimated
via a variational Bayes algorithm called *BiICE* [35] (see Fig. 2)
that imposes sparsity on the abundance vector and is based on
an appropriately defined hierarchical Bayesian model. In algorithmic form, the abundance vector can be obtained as follows:

$$x = BiICE(\Phi, y). \tag{3}$$

BilCE is computationally efficient, provides sparse solutions without requiring the fine-tuning of any parameters, and converges fast to accurate values even for highly correlated data. The determined abundance vectors x are further used for the representation of their associated pixels at the *clustering* process.

In order to unravel the advantages of using the abundance 281 representation of the pixels instead of the traditional band rep-282 resentation, we consider the following simplified case. For 283 illustration purposes, we form an RGB image selecting three 284 appropriate bands from a small area of one of the HSIs con-285 sidered in Section III-B. The considered area [see Fig. 3(a)] is 286 a class consisting of two subclasses. The representation of the 287 pixels in the original space is depicted in red color in Fig. 3(b). 288 Assuming two endmembers (one from each subclass), Fig. 3(c)289 depicts the abundance vectors stemmed from *BiICE* in blue 290 color. Note that, due to the imposed sparsity, almost all pixels 291 are concentrated around the two axes. Finally, Fig. 3(d) depicts 292 the classification map produced by SUBC. 293

It should be highlighted that the pixels in the original space 294 formulate one compact cloud with a few outliers and, thus, it 295 is difficult to be naturally divided into two separate groups. 296 On the contrary, the abundance vectors formulate two compact 297 clouds tangent to the axes, which are highly distinguished. This 298 is the advantage that characterizes the representation of the pix-299 els using their abundance vectors and eases SUBC to correctly 300 identify the two subclasses, via its second stage. It should also 301 be reminded here that the abundance vectors are characterized 302

by sparsity (i.e., the existence of zeros in vectors x), which 303 promotes data distinctions. 304

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C. Clustering

The *clustering* stage, which is applied on the abundance rep-306 resentations of the HSI pixels under study, employs the APCM 307 algorithm [30] (see Fig. 2). Let $X = \{x_i \in \Re^p, i = 1, ..., N\}$ 308 be a set of N p-dimensional data vectors to be clustered and 309 $\Theta = \{\theta_i \in \Re^p, j = 1, ..., m\}$ be a set of *m* vectors (called *rep*-310 resentatives) that will be used for the representation of the clus-311 ters formed by the points in X. Let $U = [u_{ij}], i = 1, ..., N, j =$ 312 1, ..., m be an $N \times m$ matrix whose (i, j) entry stands for the so-313 called *degree of compatibility* of x_i with the *j*th cluster denoted 314 by C_i and represented by the vector θ_i . The APCM algorithm 315 emerges from the optimization of the cost function of the origi-316 nal PCM described as follows: 317

$$J_{PCM}(\Theta, U) = \sum_{j=1}^{m} [\sum_{i=1}^{N} u_{ij} || \mathbf{x}_i - \theta_j ||^2 + \gamma_j \sum_{i=1}^{N} (u_{ij} \ln u_{ij} - u_{ij})].$$
(4)

In contrast to the classical *PCM*, where γ_j 's remain constant 318 during the execution of the algorithm, in *APCM* γ_j 's are adapted 319 at each iteration through the adaptation of the corresponding 320 η_j 's. This is achieved by setting $\gamma_j = \frac{\hat{\eta}}{\alpha} \eta_j$ and adapting η_j 321 (which is a measure of the mean absolute deviation of the current 322 form of cluster C_j) at each iteration of the algorithm. Note that 323 η_j 's and α are constant quantities (for more details see [30]). 324

The output of the algorithm is a classification map consisting 325 of clusters formed based on the abundances produced in *SU*. The 326 clusters that are formed usually correspond to regions where 327 a few abundances have high values of fractions, whereas the 328 remaining ones exhibit low values (that is, they are aggregated 329 around certain subspaces in the abundance space). 330

III. EXPERIMENTAL RESULTS AND DISCUSSION 331

SUBC has been experimentally evaluated in four case studies: 332 a synthetic and three real airborne HSI datasets of high-spatial 333 resolution. The synthetic HSI dataset has been generated with 334 various values of additive noise in order to test the sensitivity 335 of the proposed method under different noise levels. The first 336 airborne HSI dataset represents a challenging area of various 337 plant species on an agricultural area, where discrimination be-338 tween the species is impeded by numerous factors such as the 339 similar spectral signatures of the pixels as well as the absence of 340 reference spectra. The second airborne HSI dataset represents 341 a land cover of mixed vegetation and urban materials whose 342 spectral signatures patterns vary. The third airborne HSI dataset 343 represents a mainly urban area, where the spectral signatures of 344 the materials present are not characterized by specific patterns. 345

A. Synthetic HSI Dataset

The experimental evaluation of *SUBC* has been conducted on $_{347}$ a 100 \times 100 synthetic *HSI* dataset consisting of five different $_{348}$



Fig. 4. (a) Reference map of synthetic *HSI* dataset and (b) 100th band added with noise at 20 dB.



Fig. 5. Estimated abundance maps for two endmembers (a) pyroxenes and (b) carbonates extracted from synthetic *HSI* via *BiICE*. Abundance values range from 0 (blue) to 1 (red).

regions artificially generated. The spectral signatures have been 349 obtained by the U.S. Geological Survey Spectral Library [41]. 350 The data cube contains areas with mineral signatures of five 351 general mineral classes: 1) olivines; 2) pyroxenes; 3) sulfates; 352 4) oxides; and 5) carbonates. The HSI under study comprises 109 353 spectral bands. For the generation of the synthetic hyperspectral 354 data cube, seven endmembers have been randomly selected and 355 for each mineral class seven pure pixels have been assigned. 356 It should be highlighted that for each mineral class more than 357 one endmembers have been randomly assigned. Each one of the 358 five regions consists of a linear combination of different ran-359 domly selected different endmembers contaminated by additive 360 Gaussian zero mean noise. 361

Fig. 4(a) depicts the reference map, while Fig. 4(b) shows the 362 100th band of the synthetic HSI contaminated by 20-dB addi-363 tive noise. It should be noted that noise is added in all bands of 364 the synthetic HSI dataset and experiments have been conducted 365 with different SNRs in the range of 20-40 dB. Fig. 5 illustrates 366 abundance maps obtained from *BilCE* for two endmembers 1) 367 pyroxenes and 2) carbonates extracted from the synthetic HSI 368 under study. In Fig. 6, SUBC is compared with state-of-the-369 art clustering algorithms namely k-means, complete-link HAC, 370 FCM, and APCM. It should be highlighted that all these al-371 gorithms are applied on the spectral signatures of the pixels, 372 whereas the clustering procedure in SUBC is applied on the 373 abundance representations of the pixels (due to the philosophy 374 of the method). As shown in Fig. 6, classes 1, 3, and 4 are cor-375 rectly identified by all tested algorithms, while the superiority 376 of the proposed SUBC algorithm is clearly demonstrated in the 377 identification of classes 2 and 5. 378

Table I contains the results obtained by *k-means*, *HAC*, *FCM*, *APCM*, and *SUBC* in terms of *OA* and *kappa* coefficient based



Fig. 6. Clustering results emerged from: (a) *k-means*; (b) *HAC*; (c) *FCM*; (d) *APCM*; and (e) *SUBC* on the synthetic HSI under study.

 TABLE I

 COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON SYNTHETIC

 HSI DATASET IN TERMS OF OA AND Kappa Coefficient

	OA(%)	kappa
k-means	86.95	0.76
HAC	93.51	0.87
FCM	90.01	0.89
APCM	97.73	0.90
SUBC	99.28	092

TABLE II COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON SYNTHETIC HSI DATASET IN TERMS OF AA FOR EACH CLASS

Class	k-means	HAC	FCM	APCM	SUBC
1	99.76	92.51	99.70	99.72	99.78
2	77.52	93.21	77.20	97.31	98.66
3	99.24	82.24	99.30	99.25	99.26
4	75.03	99.69	85.87	99.53	99.50
5	83.20	99.90	87.98	92.84	99.20

on the obtained confusion matrix for 20-dB *SNR* [33]. Table II 381 demonstrates the results in terms of *AA* (fraction of true positives 382 and true negatives) for each class. We observe that *SUBC* outperforms all existing clustering techniques and offers an almost 384 100% *OA* and *AA*. It should be noted here that similar results 385 have also beenobtained for all other values of *SNR* tested in the range 20–40 dB. 387

B. Airborne HSI Datasets

SUBC has been also experimentally evaluated on the *HSI* 389 airborne dataset of the Salinas Valley, CA, USA [42], which 390 constitutes an arduous clustering scenario. Salinas *HSI* has been 391 collected by the Airborne Visible Infra-Red Imaging Spectrometer (*AVIRIS*) sensor over an agricultural area of Salinas 393 Valley, California. The *AVIRIS* sensor, developed by NASA's 394 Jet Propulsion Laboratory [43], generates calibrated radiance 395



Fig. 7. (a) First PCA band; (b) 117th band of Salinas Valley; and (c) masked reference map [42].

396 images in 224 contiguous spectral bands with wavelengths from 400 to 2500 nm. Moreover, it is characterized by high-spatial 397 resolution of 3.7-m pixels. The number of bands is reduced to 398 204 by removing 20 water absorption bands. Salinas Valley HSI 399 consists of vegetables and vineyard fields. Its masked reference 400 classification map comprises eight classes: corn, two types of 401 broccoli, four types of lettuce and grapes [42]. Fig. 7 depicts: 402 (a) first PCA band; (b) 117th band; and (c) masked reference 403 map of a 150×150 subimage of the Salinas Valley HSI. 404

Ideally, one would have a digital spectral library of refer-405 ence spectra of the mapped plant species. However, such a 406 publicly available library does not exist for the specific plant 407 species. In addition, it is not known how many spectra would 408 be required to represent the changing spectral signatures, as 409 a function of the growing season. This unavoidably leads to 410 the selection of the endmembers from the image itself. Doing 411 so, Fig. 8(a)-(d) depict estimated abundance maps stemmed 412 from BiICE for four endmembers extracted from Salinas Val-413 ley HSI. Fig. 8(a) and (b) correspond to two types of broccoli, 414 Fig. 8(c) to one type of grapes and Fig. 8(d) to a (most probably) 415 construction. 416

Aiming at a quantitative evaluation, SUBC is compared 417 against k-means, HAC, FCM, and APCM in terms of OA and AA 418 computed by the obtained confusion matrix as can be seen in Ta-419 bles III and IV, respectively. We see from Tables III and IV that 420 SUBC achieves OA, kappa, and AA values which are higher than 421 that of the other state-of-the-art clustering algorithms. Fig. 9 il-422 423 lustrates clustering results emerged from: (a) k-means; (b) HAC; (c) FCM; (d) APCM; and (c) SUBC on the Salinas HSI dataset. 424 It should be mentioned that the results obtained by APCM and 425 SUBC demonstrate the correct identification of all classes and 426 subclasses as can be seen by examining the first PCA band in 427 428 Fig 7(a).



Fig. 8. Estimated abundance maps for four endmembers extracted from Salinas Valley *HSI* via *BiICE*. Abundance values range from 0 (blue) to 1 (red).

TABLE III COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON SALINAS HSI DATASET IN TERMS OF OA AND Kappa Coefficient

	OA(%)	kappa
k-means	72.67	0.70
HAC	87.07	0.75
FCM	82.46	0.70
APCM	91.34	0.78
SUBC	93.04	0.80

TABLE IV Comparative Results of Clustering Algorithms on Salinas *HSI* Dataset in Terms of *AA* for Each Class

Class	k-means	HAC	FCM	APCM	SUBC
Grapes	73.67	94.27	74.92	87.92	94.77
Broccoli A	74.43	73.82	92.83	92.79	93.49
Broccoli B	73.56	73.93	90.12	90.82	91.52
Lettuce A	72.43	89.38	72.81	92.27	93.37
Lettuce B	73.21	91.59	70.62	91.39	92.36
Lettuce C	70.23	92.72	91.29	92.12	92.79
Lettuce D	71.54	93.91	92.46	93.24	93.52
Corn	72.29	86.94	74.63	90.17	92.50

SUBC has also been quantitatively evaluated on the HSI air-429 borne dataset of the Pavia Center [42]. The image has been 430 acquired by the reflective optics system imaging spectrometer 431 sensor over an urban area of the city center. The flight was 432 operated by the German Aerospace Agency under the HySens 433 project managed by the German Aerospace Center (DLR). The 434 original data consist of 115 spectral bands (with the spectral 435 range from 0.43 to 0.86 μ m) and has a high-spatial resolution of 436 1.3 m. However, noisy bands were previously removed leading 437 to a total of 102 bands. Four thematic classes are present in the 438



Fig. 9. Clustering results emerged from: (a) *k-means*; (b) *HAC*; (c) *FCM*; (d) *APCM*; and (e) *SUBC* on the Salinas *HSI*.



Fig. 10. (a) First PCA band; (b) 80th band of Pavia center; and (c) masked reference map [42] (1-yellow, 2-light blue, 3-dark blue, and 4-brown).

scene: 1) asphalt; 2) meadows; 3) trees; and 4) shadows, according to the reference classification map provided by [42]. Fig. 10 depicts: (a) first *PCA* band; (b) 80th band; and 3) masked reference map of a 300×177 subimage of the Pavia center *HSI* [42]. Fig. 11(a) and (b) depicts estimated abundance maps stemmed from *BilCE* for two endmembers: (a) shadow and (b) manmade material.

In the scope of a quantitative evaluation, *SUBC* is compared against *k-means*, *HAC*, *FCM*, and *APCM* in terms of the *OA* and *kappa* coefficient computed by the obtained confusion matrix



Fig. 11. Estimated abundance maps for two endmembers (a) shadow, (b) manmade material extracted from Pavia center *HSI* via *BiICE*. Abundance values range from 0 (blue) to 1 (red).

 TABLE V

 COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON PAVIA HSI

 DATASET IN TERMS OF OA AND Kappa Coefficient

	OA(%)	Kappa
k-means	93.26	0.80
HAC	37.03	0.71
FCM	92.46	0.78
APCM	93.38	0.79
SUBC	96.30	0.83

TABLE VI COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON PAVIA HSI DATASET IN TERMS OF AA FOR EACH CLASS

Class	k-means	HAC	FCM	APCM	SUBC
Asphalt	94.28	25.93	94.90	95.01	97.31
Meadows	90.62	16.72	92.61	91.68	96.71
Trees	92.25	21.09	86.51	90.47	94.37
Shadows	95.89	84.39	95.82	96.36	96.81

as can be seen in Table V and in terms of the *AA* as can be 449 seen in Table VI, while the clustering results of all algorithms 450 are shown in Fig. 12. Again, *SUBC* provides the best clustering 451 performance as witnessed by its *OA*, *kappa*, and *AA* values, 452 which are the highest among all its competitors. 453

Finally, SUBC has been qualitatively evaluated on the HSI 454 airborne dataset of the Washington DC mall [44]. The image 455 has been acquired by the airborne mounted Hyperspectral Dig-456 ital Imagery Collection Experiment sensor. The sensor system 457 used in this case measured pixel response in 210 bands in the 458 0.4–2.4 μ m region of the visible and infrared spectrum. Bands 459 in the 0.9–1.4 μ m region, where the atmosphere is opaque, have 460 been omitted from the dataset leaving 191 bands. Moreover, 461 the dataset exhibits high-spatial resolution (2.8 m). Five the-462 matic land cover *classes* are present in the scene: 1) roof; 2) 463 grass; 3) trees; 4) water; and 5) asphalt road, according to the 464



Fig. 12. Clustering results emerged from: (a) *k-means*, (b) *HAC*, (c) *FCM*, (d) *APCM* and (e) *SUBC* on the Pavia center *HSI*.



Fig. 13. (a) First PCA band; (b) 100th band of Washington DC; and (c) reference map [44].

classification map provided by [49] and used here as a referencemap.

Fig. 13 depicts: (a) first *PCA* band; (b) 100th band; and (c) reference map of a 100×100 subimage of the Washington DC mall *HSI* [44]. It should be noticed that the reference map is provided only for qualitative visualization assessment and it is not accurate for a thorough quantitative assessment. Fig. 14(a)



Fig. 14. Estimated abundance maps for two endmembers: (a) manmade material and(b) (most probably) soil/grass of class 1 extracted from Washington DC HSI via BiICE. Abundance values range from 0 (blue) to 1 (red).



Fig. 15. Clustering results emerged from: (a) k-means; (b) HAC; (c) FCM; (d) APCM; and (e) SUBC on the Washington DC HSI.

and (b) depicts estimated abundance maps stemmed from *Bi*-472 *ICE* for two endmembers: 1) manmade material and 2) (most 473 probably) soil/grass of class 1. Fig. 15 illustrates clustering results emerged from: (a) *k-means*; (b) *HAC*; (c) *FCM*; (d) *APCM*; 475 and (e) *SUBC* on the Washington DC *HSI* dataset. It should be highlighted that, apart from *SUBC*, all other algorithms falsely classify water and asphalt road pixels to one class. On the other hand, *SUBC* correctly distinguishes pixels that belong to the water class from all other pixels that belong to the remaining classes. 481

As it has been highlighted throughout the paper, the key idea 482 of the proposed method is to perform unmixing at its first stage, 483 in order to take the abundance representations of the pixels 484 and then, at the second stage, to perform clustering based on 485 the pixels abundance vector representations. Clearly, one could 486 choose any unmixing method in the first stage and any clustering 487 method in the second stage of the algorithm. In order to justify 488 the choice of *BiICE* in the first stage, we compare it against 489 two AE algorithms: 1) a quadratic programming (QP) technique 490 [45], which does not exploit sparsity and 2) the sparse unmix-491 ing by variable splitting and augmented Lagrangian (SUnSAL) 492 algorithm [46], which, as *BiICE*, imposes sparsity. That is, we 493 substitute *BiICE* with *QP* and *SUnSAL* at the first stage of the 494 proposed method. Leaned on Table VII, which depicts the OA 495

TABLE VII COMPARATIVE RESULTS OF SU ALGORITHMS ON HSI DATASETS IN TERMS OF OA

	Synthetic	Salinas	Pavia
QP	83.67	74.32	71.20
SUnSAL BiICE	97.50 99.28	82.71 93.04	87.52 96.30

of the three cases, the QP algorithm attains the worst perfor-496 mance (since it does not take into account that by the nature of 497 the problem, the abundance vectors exhibit sparsity), whereas 498 499 SUnSAL exhibits significantly improved performance compared to QP, yet inferior, compared to BiICE, especially for real data. 500 Moreover, SUnSAL comes at the additional expense of manually 501 fine-tuning nontrivial parameters, such as a sparsity promoting 502 parameter λ . 503

The choice of APCM in the second stage of the algorithm is 504 505 justified mainly by the fact that it is able to estimate automatically the underlying number of clusters in the dataset. Moreover, 506 focusing on the first four lines of Tables I, III, and IV, the OA 507 of APCM is significantly higher from all other state of the art 508 clustering methods (note that all these algorithms are applied on 509 510 the same dataset, i.e., the spectral signature representations of the HSI pixels). 511

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IV. CONCLUSION AND FUTURE DIRECTIONS

The key challenge of the proposed method (SUBC) is the iden-513 tification of spatially homogeneous regions comprising different 514 materials. The method consists of two main stages (unmixing 515 and clustering) and generates three significant (by)products, 516 namely: 1) endmembers; 2) abundance vectors (abundance 517 maps); and 3) clusters (classification maps). The key feature of 518 SUBC is the utilization of the abundance representations of the 519 HSI pixels (as they result from the unmixing stage) in the cluster-520 ing stage. The advantage of using the abundance representation 521 instead of the basic spectral representation of the pixels is that 522 the former, in contrast to the latter, provides subpixel level infor-523 mation, which in turn favors more detailed classification maps. 524 Moreover, the abundance representation is likely to give rise to 525 more well-discriminated clusters that live on subspaces of the 526 abundance space, due to the fact that only a few materials are 527 expected to contribute to the formation of a HSI pixel (sparsity 528 issue). As a consequence, subspace clustering algorithms could 529 also be considered as an alternative in the final stage of the algo-530 rithm, since the abundance representations are likely to lead to 531 532 clusters that live to subspaces of the abundance space. SUBC is unsupervised and does not require class information knowledge 533 of the dataset under study. Moreover, it is image independent, 534 it alleviates the "curse of dimensionality" issue and enhances 535 localization and accuracy since it operates in the subpixel level 536 of information. However, it is noted again that the correct iden-537 tification of the endmembers number and their correspondence 538 539 to physical objects/materials is undoubtedly the most critical

step for successful SU and, as a consequence, for the clustering 540 processes. 541

Experimental results show that *SUBC* compares favorably to 542 other related methods. This gives us confidence to claim that the 543 performance of the proposed method remains consistent with 544 high-spatial resolution airborne data. It is capable of identifying 545 compact regions and spectral regions that lack training data. 546

In terms of future directions, the full potential of this al-547 gorithm will be investigated with additional hyperspectral ac-548 quisitions of higher mixture complexity. In addition, this study 549 could be reinforced and expanded in the case of existing and 550 future satellite hypespectral data imagery of lower spatial res-551 olutions where increased complexity issues for the tasks of 1) 552 endmember identification; 2) resolving shadowing effects; and 553 3) facing oblique viewing and illumination angles arise. More-554 over, subspace clustering algorithms could be utilized, since as 555 we discussed earlier, they suit nicely in the nature of the problem 556 in the abundance space. 557

ACKNOWLEDGMENT

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The AVIRIS data were provided courtesy of NASA/JPL-559 Caltech in Pasadena, CA, USA, via the EXELIS Visual In-560 formation Solutions Inc., 2012. 561

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720Dr. Mylona received a scholarship co-financed by the European Union and
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Dr. Mylona received a scholarship co-financed by the European Union and Greek national funds through the research funding program Heracleitus II.



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Spectral Unmixing-Based Clustering of High-Spatial Resolution Hyperspectral Imagery

Eleftheria A. Mylona, Olga A. Sykioti, Konstantinos D. Koutroumbas, and Athanasios A. Rontogiannis, *Member, IEEE*

Abstract—This paper introduces a novel unsupervised spectral 5 unmixing-based clustering method for high-spatial resolution hy-6 7 perspectral images (HSIs). In contrast to most clustering methods reported so far, which are applied on the spectral signature repre-8 9 sentations of the image pixels, the idea in the proposed method is to apply clustering on the abundance representations of the pixels. 10 Specifically, the proposed method comprises two main processing 11 stages namely: an unmixing stage (consisting of the endmember 12 extraction and abundance estimation (AE) substages) and a clus-13 tering stage. In the former stage, suitable endmembers are selected 14 first as the most representative pure pixels. Then, the spectral sig-15 nature of each pixel is expressed as a linear combination of the 16 17 endmembers' spectral signatures and the pixel itself is represented by the relative abundance vector, which is estimated via an efficient 18 AE algorithm. The resulting abundance vectors associated with the 19 20 HSI pixels are next fed to the clustering stage. Eventually, the pixels are grouped into clusters, in terms of their associated abundance 21 22 vectors and not their spectral signatures. Experiments are per-23 formed on a synthetic HSI dataset as well as on three airborne 24 HSI datasets of high-spatial resolution containing vegetation and 25 urban areas. The experimental results corroborate the effective-26 ness of the proposed method and demonstrate that it outperforms state-of-the-art clustering techniques in terms of overall accuracy, 27 average accuracy, and kappa coefficient. 28

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Index Terms—Abundance estimation (AE), clustering, endmember extraction (EE), hyperspectral imagery (HSI), spectral unmixing (SU).

I. INTRODUCTION

H YPERSPECTRAL imaging has enabled applications and detailed mapping possibilities in a wide variety of Earth studies. In particular, airborne hyperspectral images (*HSIs*) offer high-spatial resolution with detailed spectral accuracy. This versatility enhances the identification, modeling, and detailed classification of various natural and man-made materials. *HSIs* are collected via hyperspectral sensors and are represented as data cubes consisting of numerous contiguous spectral bands of narrow bandwidths. A significant characteristic of *HSIs*, which

Manuscript received September 14, 2016; revised November 21, 2016 and January 24, 2017; accepted March 13, 2017. Manuscript received September 14, 2016. This work was supported by the PHySIS Project under Contract 640174 within the H2020 Framework Program of the European Commission. (*Corresponding author: Eleftheria A. Mylona.*)

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Digital Object Identifier 10.1109/JSTARS.2017.2687703

makes their processing more challenging, is the presence of 42 *mixed pixels*, which depict surface regions consisting of two or 43 more distinct materials. The data for each mixed pixel corre-44 spond to the total reflectance of all the materials present within 45 the pixel in numerous spectral bands from the surface depicted 46 by the pixel, which form the *spectral signature* of the pixel. 47 The key objectives in HSI processing are: 1) the detection of 48 the constituent components of mixed HSI pixels as well as the 49 proportions in which they appear, which will allow the produc-50 tion of abundance maps per material and 2) the identification 51 of spectrally homogeneous regions. The first objective is tack-52 led via spectral unmixing (SU) and the second via the use of 53 clustering algorithms. 54

In this study, we focus on the problem of identifying spec-55 trally homogeneous regions, via clustering (unsupervised) tech-56 niques, which, in contrast to their supervised counterparts, they 57 do not require any externally labeled set of pixels. Most cluster-58 ing techniques proposed in this field are applied on the spectral 59 signature representations of the pixels. In contrast, the key idea 60 of the proposed methodology is to apply clustering on the abun-61 dance vector representations of the HSI pixels, since the latter 62 representation is likely to lead to more well-separated clusters. 63 To this end, SU is applied first on the spectral representations 64 of the pixels, in order to extract the corresponding abundance 65 vectors, and then, clustering is applied on the abundance vector 66 pixels representations. 67

SU [1]–[6] of HSIs has been widely applied to environmental 68 studies. It consists of two main substages, namely 1) endmem-69 ber extraction and 2) abundance estimation (AE). EE [7]-[11] is 70 a challenging process since the aim is to mine the purest pixels 71 (endmembers) of each spectrally distinct material of a HSI. The 72 latter almost always consists of mixed pixels, which are also af-73 fected by noise spectra. Ideally, each endmember ought to have 74 the maximum possible abundance of a single physical material 75 present in the HSI under study and minimum (close to zero) 76 abundance for the rest of the physical materials. Moreover, the 77 determination of the number of endmembers is critical since an 78 underestimated number may result in poor representation of the 79 mixed HSI pixels under study, whereas an overestimated num-80 ber may comprise a lot of mixed signatures. Popular endmember 81 extraction algorithms (EEAs) include VCA [12], N-FINDR vari-82 ants [13], and MVSA [14]. Other related algorithms are discussed 83 in [16]–[18]. 84

The aim of *AE* is the decomposition of the spectral signatures of mixed pixels into a selection of spectral signatures

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corresponding to the reflectance of pure physical materials (end-87 *members*). The latter is usually extracted by the image itself via 88 EE (however, in some cases they are selected from specific 89 90 spectral libraries). AE results in a set of corresponding fractions (abundances), which indicate the proportion of each endmem-91 ber present in a given pixel. Clearly, the ultimate success of AE 92 depends heavily on the appropriate selection of endmembers. 93 Since only a small number of the available materials' spectra 94 are expected to be present in a HSI pixel (especially in high-res-95 96 olution HSIs), the abundance vectors are expected to be sparse. Clustering [19], [20] partitions a set of pixels from the input 97 image into groups. Some of the most known clustering ap-98 proaches are the k-means [21], the Fuzzy C-Means (FCM) [22], 99 the Possibilistic C-Means (PCM) [23] and their variants, e.g., 100 [24], [25]. The aforementioned algorithms are suitable for re-101 covering compact clusters and they use specific vectors, (called 102 representatives) to represent the clusters that underlie in the 103 current dataset. In contrast to these algorithms, that provide a 104 single data clustering, in Hierarchical Agglomerative Clustering 105 (HAC) [26], [27], the data are organized into an effective hier-106 107 archy of nested clusterings. HAC requires a metric in order to calculate the dissimilarity between pairs of pixels and a linkage 108 so as to measure the dissimilarity between clusters. 109

110 A. Related Work

It should be mentioned that the literature on clustering tech-111 niques applied on HSIs is limited. In [28], a graph data struc-112 ture is generated to represent the tree crowns weighted with 113 114 the Euclidean distance. A minimum spanning tree is generated using Kruskal's algorithm and edges above a length threshold 115 are removed to generate independent clusters. In [29], an unsu-116 pervised hierarchical cluster analysis to phytoplankton pigment 117 data is applied with the aim of discriminating different phy-118 toplankton assemblages in open ocean environments. Several 119 types of optical data vectors are used as input to HAC including 120 objects consisting of reflectance values of hyperspectral data. 121 Also, in [30], a new clustering algorithm, named Adaptive Pos-122 sibilistic C-Means (APCM), is applied on HSIs. 123

In [31], a clustering procedure is proposed, which consists of 124 three processes: 1) EE, 2) unmixing and 3) hardening process 125 via the winner-takes-all approach, in order to produce recon-126 structed pixels spectra. In [32], the proposed work utilizes the 127 Gauss Mixture Vector Quantization algorithm to learn the mix-128 ture analysis and explores the cluster analysis with correlation 129 distance. In [33], SU is combined with k-means cluster analysis 130 for accurate geological mapping. The data are first classified 131 into two categories: hydrothermal alteration areas and unal-132 tered rocks. SU is applied to hydrothermal alteration areas and 133 134 k-means clustering to unaltered rocks as two separate approaches. In [34], the proposed work generates classification 135 maps based on k-means clustering and Gradient Flow. SU is 136 conducted using the Max-D algorithm to automatically find 137 endmembers. It should be highlighted that, in all previous meth-138 ods, the unmixing and clustering processes are utilized as two 139 separate steps, in the sense that their results are extracted inde-140 141 pendently from each other and are combined next.

In this paper, a novel unsupervised SU-based clustering 142 method (SUBC) for HSIs is proposed. SUBC consists of two 143 processing stages namely: 1) SU, which consists of an EEA, 144 followed by a (sparse) AE algorithm and 2) a clustering algo-145 rithm. The first process identifies suitable endmembers based 146 on the VCA algorithm [12]. Then, AE is applied on each image 147 pixel, in order to provide its abundance representation, using the 148 sparsity-promoting *BiICE* algorithm [35]. Finally, the recently 149 proposed APCM clustering algorithm [30] uses the abundance 150 representations of the pixels, in order to group them into clus-151 ters. It should be noted that the abundance pixel representations 152 adopted in the proposed methodology ensures (in general) a 153 common sparsity pattern for pixels in the same cluster. To the 154 best of our knowledge, this is the first attempt of utilizing the 155 abundance representation of pixels generated by SU as input to 156 a clustering algorithm with the aim to enhance classification in 157 HSIs. 158

The proposed *SUBC* method is evaluated on a synthetic *HSI* 159 dataset as well as on three airborne *HSI* datasets of high-spatial 160 resolution (the agricultural area of Salinas Valley, CA, USA, the 161 land cover at Washington DC Mall, USA, and the urban area of 162 the Pavia center, Italy) and its performance is compared in terms 163 of overall accuracy (*OA*), average accuracy (*AA*) and kappa 164 coefficient with that of state-of-the-art clustering techniques. 165

The paper is organized as follows. Section II introduces the proposed *SUBC* method. Section III demonstrates the results obtained by the proposed method as well as comparisons with state-of-the-art clustering algorithms. Conclusion and future research directions are summarized in Section IV. 170

II. PROPOSED SUBC METHOD

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In this section, we first present the motivation and contribution of this study and then we describe in detail the proposed 173 unmixing-based clustering algorithm. 174

A. Motivation and Contribution

In general, classification algorithms [36], [37] (both super-176 vised and unsupervised) developed so far are applied directly on 177 the *L*-dimensional spectral band vectors of the pixels. However, 178 such (usually high dimensional) representations may contain a 179 lot of redundant information, which may cause pixels depicting 180 different areas to be not well separated from each other in the 181 *L*-dimensional spectral domain. Clearly, this renders the work 182 of the classification algorithms more difficult. Apart from the 183 above issue, most classification schemes used for HSI processing 184 do not focus on exploiting the available fine spectral resolution, 185 that is, they do not consider at all information within the pixel. A 186 further consequence of this is that such schemes do not exploit 187 the fact that each *HSI* pixel contains only a few of the materials 188 existing in the whole HSI (equivalently, the spectral signature of 189 each pixel is expected to result from the linear combination of 190 only a few endmember spectral signatures, which implies that 191 the corresponding abundance vectors will be *sparse*). 192

The approach that we adopt in this paper in order to leverage 193 the above issues is to employ sparsity-promoting SU techniques 194 in order to represent each pixel by its abundance vector (with 195



Fig. 1. Conceptual illustration of the dimensionality reduction achieved, moving from the original band space (usually consisting of hundreds of spectral bands) to the "less correlated" low-dimensional abundance space.

respect to a set of endmembers) and not by its spectral sig-196 197 nature. The rationale behind this choice is twofold. First, the dimension of the abundance vector space (which equals to the 198 199 number of the endmembers depicted in the HSI under study) is usually much lower than the dimension of the spectral signature 200 space (number of spectral bands) (see Fig. 1). Since the cor-201 responding original feature space (the space where each band 202 defines an axis) is high dimensional, the Hughes phenomenon 203 [38] ("curse" of dimensionality) appears. In light of this, the 204 original high-dimensional space of the HSI is transformed to 205 the dimensionally reduced space of abundance vectors [39]. 206

Second, assuming that the endmembers are pure pixels, the 207 (sparse) abundance vectors are expected to form clusters, which 208 209 are likely to lie in different subspaces in the abundance space. It is, thus, anticipated that different classes will form more easily 210 distinguishable clusters in the abundance vectors space. Gener-211 ally speaking, adoption of the abundance representation is ex-212 pected to ease the work of the classification methods. However, 213 214 we have to keep in mind that the abundance retrieval requires a very good estimation of the endmembers that have a physical 215 meaning in order to work properly, which, in practice, is not 216 straightforward. 217

In the SU stage of the SUBC an EEA is first employed, which 218 identifies appropriate endmembers of the image. Next, a sparse 219 220 AE algorithm is used that is based on the endmembers extracted by the EEA, in order to produce the abundance fractions for 221 each pixel, which in turn form the abundance vector of the 222 pixel. These vectors of all pixels are fed to the second stage of 223 the SUBC method, where a clustering algorithm groups pixels 224 225 based on their abundance representations.

An additional feature concerning the mapping to the abun-226 dance space that should be highlighted is that the number of 227 clusters and the number of endmembers are (in general) dif-228 ferent. A cluster formed according to the abundances usually 229 corresponds to a region where a single (or a few) endmembers 230 have high proportion, whereas all other endmembers have low 231 proportions. However, it can also correspond to the mixture of 232 several endmembers of varied proportions. The block diagram 233 of SUBC is depicted in Fig. 2. 234

235 B. Spectral Unmixing

236 1) Endmember Extraction: Aiming at detecting suitable 237 endmembers, we utilize the *VCA* algorithm [12], which takes



Fig. 2. Block diagram of SUBC.

as input the spectral signatures of the pixels, as can be seen in 238 Fig. 2. Each pixel can be viewed as a vector in an L-dimensional 239 Euclidean space, where each spectral band is assigned to one 240 axis of the space. Based on the aforesaid data points, the 241 VCA algorithm returns a prespecified number of endmembers 242 via iteratively projecting data onto a direction orthogonal to 243 the subspace spanned by the endmembers already determined. 244 The new endmember signature corresponds to the extreme 245 of the projection. The algorithm iterates until the number of 246 endmembers is exhausted [12]. Then, SUBC continues in esti-247 mating the abundance fractions of each endmember via AE. 248

2) Abundance Estimation: The selection of appropriate endmembers is crucial so as to correctly estimate the abundance
fractions. Usually, the spectral signature of the pixel, denoted
by *y*, is assumed to follow the Linear Mixing Model [40] according to which it can be expressed as a linear combination of
its endmembers' spectra as follows:

$$y = \Phi x + n \tag{1}$$

where $\Phi = [\varphi_1, \varphi_2, ..., \varphi_p] \in \Re_+^{L \times p}$, $L \gg p$, is the mixing matrix comprising the endmembers' spectra (*L*-dimensional vectors ϕ_i , i = 1, 2, ..., p), \mathbf{x} is a $p \times 1$ vector consisting of the 257 corresponding abundance fractions, named *abundance vector*, 258 and \mathbf{n} is an $L \times 1$ additive noise vector, which is assumed to be 259 a zero-mean Gaussian distributed random vector with independent and identically distributed elements. 261

Due to the physical constraints of the unmixing problem, the 262 abundance fractions for each pixel should satisfy the following 263 two constraints: 264

$$x_i \ge 0, \ i = 1, \ 2, \ ..., \ N, \quad \sum_{i=1}^N x_i = 1$$
 (2)

that is, the abundances should be nonnegative and they must 265 sum to 1. Furthermore, the *abundance* vector is expected to be 266 sparse, i.e., only a few of its elements will be nonzero, since the 267

Fig. 3. (a) Class of the *HSI* containing two subclasses; (b) representation of pixels in the original space; (c) representation of abundance vectors $x = x_1, x_2$; and (d) clustering result emerged from *SUBC*.

area depicted by a single pixel is likely to embed only a small
fraction of the different materials encountered in the whole *HSI*.
In this study, the abundance vector for each pixel is estimated
via a variational Bayes algorithm called *BiICE* [35] (see Fig. 2)
that imposes sparsity on the abundance vector and is based on
an appropriately defined hierarchical Bayesian model. In algorithmic form, the abundance vector can be obtained as follows:

$$x = BiICE(\Phi, y). \tag{3}$$

BilCE is computationally efficient, provides sparse solutions without requiring the fine-tuning of any parameters, and converges fast to accurate values even for highly correlated data. The determined abundance vectors x are further used for the representation of their associated pixels at the *clustering* process.

In order to unravel the advantages of using the abundance 281 representation of the pixels instead of the traditional band rep-282 resentation, we consider the following simplified case. For 283 illustration purposes, we form an RGB image selecting three 284 appropriate bands from a small area of one of the HSIs con-285 sidered in Section III-B. The considered area [see Fig. 3(a)] is 286 a class consisting of two subclasses. The representation of the 287 pixels in the original space is depicted in red color in Fig. 3(b). 288 Assuming two endmembers (one from each subclass), Fig. 3(c)289 depicts the abundance vectors stemmed from BiICE in blue 290 color. Note that, due to the imposed sparsity, almost all pixels 291 are concentrated around the two axes. Finally, Fig. 3(d) depicts 292 the classification map produced by SUBC. 293

It should be highlighted that the pixels in the original space 294 formulate one compact cloud with a few outliers and, thus, it 295 is difficult to be naturally divided into two separate groups. 296 On the contrary, the abundance vectors formulate two compact 297 clouds tangent to the axes, which are highly distinguished. This 298 is the advantage that characterizes the representation of the pix-299 els using their abundance vectors and eases SUBC to correctly 300 identify the two subclasses, via its second stage. It should also 301 be reminded here that the abundance vectors are characterized 302

by sparsity (i.e., the existence of zeros in vectors x), which 303 promotes data distinctions. 304

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C. Clustering

The *clustering* stage, which is applied on the abundance rep-306 resentations of the HSI pixels under study, employs the APCM 307 algorithm [30] (see Fig. 2). Let $X = \{x_i \in \Re^p, i = 1, ..., N\}$ 308 be a set of N p-dimensional data vectors to be clustered and 309 $\Theta = \{\theta_i \in \Re^p, j = 1, ..., m\}$ be a set of *m* vectors (called *rep*-310 resentatives) that will be used for the representation of the clus-311 ters formed by the points in X. Let $U = [u_{ij}], i = 1, ..., N, j =$ 312 1, ..., m be an $N \times m$ matrix whose (i, j) entry stands for the so-313 called *degree of compatibility* of x_i with the *j*th cluster denoted 314 by C_i and represented by the vector θ_i . The APCM algorithm 315 emerges from the optimization of the cost function of the origi-316 nal PCM described as follows: 317

$$J_{PCM}(\Theta, U) = \sum_{j=1}^{m} \left[\sum_{i=1}^{N} u_{ij} || \mathbf{x}_i - \theta_j ||^2 + \gamma_j \sum_{i=1}^{N} (u_{ij} \ln u_{ij} - u_{ij}) \right].$$
(4)

In contrast to the classical *PCM*, where γ_j 's remain constant 318 during the execution of the algorithm, in *APCM* γ_j 's are adapted 319 at each iteration through the adaptation of the corresponding 320 η_j 's. This is achieved by setting $\gamma_j = \frac{\hat{\eta}}{\alpha} \eta_j$ and adapting η_j 321 (which is a measure of the mean absolute deviation of the current 322 form of cluster C_j) at each iteration of the algorithm. Note that 323 η_j 's and α are constant quantities (for more details see [30]). 324

The output of the algorithm is a classification map consisting 325 of clusters formed based on the abundances produced in *SU*. The 326 clusters that are formed usually correspond to regions where 327 a few abundances have high values of fractions, whereas the 328 remaining ones exhibit low values (that is, they are aggregated 329 around certain subspaces in the abundance space). 330

III. EXPERIMENTAL RESULTS AND DISCUSSION 331

SUBC has been experimentally evaluated in four case studies: 332 a synthetic and three real airborne HSI datasets of high-spatial 333 resolution. The synthetic HSI dataset has been generated with 334 various values of additive noise in order to test the sensitivity 335 of the proposed method under different noise levels. The first 336 airborne HSI dataset represents a challenging area of various 337 plant species on an agricultural area, where discrimination be-338 tween the species is impeded by numerous factors such as the 339 similar spectral signatures of the pixels as well as the absence of 340 reference spectra. The second airborne HSI dataset represents 341 a land cover of mixed vegetation and urban materials whose 342 spectral signatures patterns vary. The third airborne HSI dataset 343 represents a mainly urban area, where the spectral signatures of 344 the materials present are not characterized by specific patterns. 345

A. Synthetic HSI Dataset

The experimental evaluation of *SUBC* has been conducted on $_{347}$ a 100 \times 100 synthetic *HSI* dataset consisting of five different $_{348}$





Fig. 4. (a) Reference map of synthetic HSI dataset and (b) 100th band added with noise at 20 dB.



Fig. 5. Estimated abundance maps for two endmembers (a) pyroxenes and (b) carbonates extracted from synthetic *HSI* via *BiICE*. Abundance values range from 0 (blue) to 1 (red).

regions artificially generated. The spectral signatures have been 349 obtained by the U.S. Geological Survey Spectral Library [41]. 350 The data cube contains areas with mineral signatures of five 351 general mineral classes: 1) olivines; 2) pyroxenes; 3) sulfates; 352 4) oxides; and 5) carbonates. The HSI under study comprises 109 353 354 spectral bands. For the generation of the synthetic hyperspectral data cube, seven endmembers have been randomly selected and 355 for each mineral class seven pure pixels have been assigned. 356 It should be highlighted that for each mineral class more than 357 one endmembers have been randomly assigned. Each one of the 358 five regions consists of a linear combination of different ran-359 domly selected different endmembers contaminated by additive 360 Gaussian zero mean noise. 361

Fig. 4(a) depicts the reference map, while Fig. 4(b) shows the 362 100th band of the synthetic HSI contaminated by 20-dB addi-363 tive noise. It should be noted that noise is added in all bands of 364 the synthetic HSI dataset and experiments have been conducted 365 with different SNRs in the range of 20-40 dB. Fig. 5 illustrates 366 abundance maps obtained from *BilCE* for two endmembers 1) 367 pyroxenes and 2) carbonates extracted from the synthetic HSI 368 under study. In Fig. 6, SUBC is compared with state-of-the-369 art clustering algorithms namely k-means, complete-link HAC, 370 FCM, and APCM. It should be highlighted that all these al-371 gorithms are applied on the spectral signatures of the pixels, 372 whereas the clustering procedure in SUBC is applied on the 373 abundance representations of the pixels (due to the philosophy 374 of the method). As shown in Fig. 6, classes 1, 3, and 4 are cor-375 rectly identified by all tested algorithms, while the superiority 376 of the proposed SUBC algorithm is clearly demonstrated in the 377 identification of classes 2 and 5. 378

Table I contains the results obtained by *k-means*, *HAC*, *FCM*, *APCM*, and *SUBC* in terms of *OA* and *kappa* coefficient based



Fig. 6. Clustering results emerged from: (a) *k-means*; (b) *HAC*; (c) *FCM*; (d) *APCM*; and (e) *SUBC* on the synthetic HSI under study.

TABLE I COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON SYNTHETIC HSI DATASET IN TERMS OF OA AND Kappa Coefficient

	OA(%)	kappa
k-means	86.95	0.76
HAC	93.51	0.87
FCM	90.01	0.89
APCM	97.73	0.90
SUBC	99.28	092

TABLE II COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON SYNTHETIC HSI DATASET IN TERMS OF AA FOR EACH CLASS

Class	k-means	HAC	FCM	APCM	SUBC
1	99.76	92.51	99.70	99.72	99.78
2	77.52	93.21	77.20	97.31	98.66
3	99.24	82.24	99.30	99.25	99.26
4	75.03	99.69	85.87	99.53	99.50
5	83.20	99.90	87.98	92.84	99.20

on the obtained confusion matrix for 20-dB *SNR* [33]. Table II 381 demonstrates the results in terms of *AA* (fraction of true positives 382 and true negatives) for each class. We observe that *SUBC* outperforms all existing clustering techniques and offers an almost 384 100% *OA* and *AA*. It should be noted here that similar results 385 have also beenobtained for all other values of *SNR* tested in the range 20–40 dB. 387

B. Airborne HSI Datasets

SUBC has been also experimentally evaluated on the *HSI* 389 airborne dataset of the Salinas Valley, CA, USA [42], which 390 constitutes an arduous clustering scenario. Salinas *HSI* has been 391 collected by the Airborne Visible Infra-Red Imaging Spectrometer (*AVIRIS*) sensor over an agricultural area of Salinas 393 Valley, California. The *AVIRIS* sensor, developed by NASA's 394 Jet Propulsion Laboratory [43], generates calibrated radiance 395



Fig. 7. (a) First PCA band; (b) 117th band of Salinas Valley; and (c) masked reference map [42].

396 images in 224 contiguous spectral bands with wavelengths from 400 to 2500 nm. Moreover, it is characterized by high-spatial 397 resolution of 3.7-m pixels. The number of bands is reduced to 398 204 by removing 20 water absorption bands. Salinas Valley HSI 399 consists of vegetables and vineyard fields. Its masked reference 400 classification map comprises eight classes: corn, two types of 401 402 broccoli, four types of lettuce and grapes [42]. Fig. 7 depicts: (a) first PCA band; (b) 117th band; and (c) masked reference 403 map of a 150×150 subimage of the Salinas Valley HSI. 404

Ideally, one would have a digital spectral library of refer-405 ence spectra of the mapped plant species. However, such a 406 publicly available library does not exist for the specific plant 407 species. In addition, it is not known how many spectra would 408 be required to represent the changing spectral signatures, as 409 a function of the growing season. This unavoidably leads to 410 the selection of the endmembers from the image itself. Doing 411 so, Fig. 8(a)-(d) depict estimated abundance maps stemmed 412 from BiICE for four endmembers extracted from Salinas Val-413 ley HSI. Fig. 8(a) and (b) correspond to two types of broccoli, 414 Fig. 8(c) to one type of grapes and Fig. 8(d) to a (most probably) 415 construction. 416

Aiming at a quantitative evaluation, SUBC is compared 417 against k-means, HAC, FCM, and APCM in terms of OA and AA 418 computed by the obtained confusion matrix as can be seen in Ta-419 bles III and IV, respectively. We see from Tables III and IV that 420 SUBC achieves OA, kappa, and AA values which are higher than 421 that of the other state-of-the-art clustering algorithms. Fig. 9 il-422 lustrates clustering results emerged from: (a) k-means; (b) HAC; 423 (c) FCM; (d) APCM; and (c) SUBC on the Salinas HSI dataset. 424 It should be mentioned that the results obtained by APCM and 425 SUBC demonstrate the correct identification of all classes and 426 subclasses as can be seen by examining the first PCA band in 427 428 Fig 7(a).



Fig. 8. Estimated abundance maps for four endmembers extracted from Salinas Valley *HSI* via *BiICE*. Abundance values range from 0 (blue) to 1 (red).

 TABLE III

 COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON SALINAS

 HSI DATASET IN TERMS OF OA AND Kappa Coefficient

	OA(%)	kappa
k-means	72.67	0.70
HAC	87.07	0.75
FCM	82.46	0.70
APCM	91.34	0.78
SUBC	93.04	0.80

TABLE IV Comparative Results of Clustering Algorithms on Salinas *HSI* Dataset in Terms of *AA* for Each Class

Class	k-means	HAC	FCM	APCM	SUBC
Grapes	73.67	94.27	74.92	87.92	94.77
Broccoli A	74.43	73.82	92.83	92.79	93.49
Broccoli B	73.56	73.93	90.12	90.82	91.52
Lettuce A	72.43	89.38	72.81	92.27	93.37
Lettuce B	73.21	91.59	70.62	91.39	92.36
Lettuce C	70.23	92.72	91.29	92.12	92.79
Lettuce D	71.54	93.91	92.46	93.24	93.52
Corn	72.29	86.94	74.63	90.17	92.50

SUBC has also been quantitatively evaluated on the HSI air-429 borne dataset of the Pavia Center [42]. The image has been 430 acquired by the reflective optics system imaging spectrometer 431 sensor over an urban area of the city center. The flight was 432 operated by the German Aerospace Agency under the HySens 433 project managed by the German Aerospace Center (DLR). The 434 original data consist of 115 spectral bands (with the spectral 435 range from 0.43 to 0.86 μ m) and has a high-spatial resolution of 436 1.3 m. However, noisy bands were previously removed leading 437 to a total of 102 bands. Four thematic classes are present in the 438







Fig. 10. (a) First PCA band; (b) 80th band of Pavia center; and (c) masked reference map [42] (1-yellow, 2-light blue, 3-dark blue, and 4-brown).

scene: 1) asphalt; 2) meadows; 3) trees; and 4) shadows, according to the reference classification map provided by [42]. Fig. 10 depicts: (a) first *PCA* band; (b) 80th band; and 3) masked reference map of a 300×177 subimage of the Pavia center *HSI* [42]. Fig. 11(a) and (b) depicts estimated abundance maps stemmed from *BilCE* for two endmembers: (a) shadow and (b) manmade material.

In the scope of a quantitative evaluation, *SUBC* is compared against *k-means*, *HAC*, *FCM*, and *APCM* in terms of the *OA* and *kappa* coefficient computed by the obtained confusion matrix



Fig. 11. Estimated abundance maps for two endmembers (a) shadow, (b) manmade material extracted from Pavia center *HSI* via *BiICE*. Abundance values range from 0 (blue) to 1 (red).

 TABLE V

 COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON PAVIA HSI

 DATASET IN TERMS OF OA AND Kappa Coefficient

	OA(%)	Kappa
k-means	93.26	0.80
HAC	37.03	0.71
FCM	92.46	0.78
APCM	93.38	0.79
SUBC	96.30	0.83

TABLE VI COMPARATIVE RESULTS OF CLUSTERING ALGORITHMS ON PAVIA HSI DATASET IN TERMS OF AA FOR EACH CLASS

Class	k-means	HAC	FCM	APCM	SUBC
Asphalt	94.28	25.93	94.90	95.01	97.31
Meadows	90.62	16.72	92.61	91.68	96.71
Trees	92.25	21.09	86.51	90.47	94.37
Shadows	95.89	84.39	95.82	96.36	96.81

as can be seen in Table V and in terms of the *AA* as can be 449 seen in Table VI, while the clustering results of all algorithms 450 are shown in Fig. 12. Again, *SUBC* provides the best clustering 451 performance as witnessed by its *OA*, *kappa*, and *AA* values, 452 which are the highest among all its competitors. 453

Finally, SUBC has been qualitatively evaluated on the HSI 454 airborne dataset of the Washington DC mall [44]. The image 455 has been acquired by the airborne mounted Hyperspectral Dig-456 ital Imagery Collection Experiment sensor. The sensor system 457 used in this case measured pixel response in 210 bands in the 458 0.4–2.4 μ m region of the visible and infrared spectrum. Bands 459 in the 0.9–1.4 μ m region, where the atmosphere is opaque, have 460 been omitted from the dataset leaving 191 bands. Moreover, 461 the dataset exhibits high-spatial resolution (2.8 m). Five the-462 matic land cover *classes* are present in the scene: 1) roof; 2) 463 grass; 3) trees; 4) water; and 5) asphalt road, according to the 464

(a)

Fig. 14. Estimated abundance maps for two endmembers: (a) manmade material and(b) (most probably) soil/grass of class 1 extracted from Washington DC HSI via BiICE. Abundance values range from 0 (blue) to 1 (red).

(b)

Fig. 15. Clustering results emerged from: (a) k-means; (b) HAC; (c) FCM; (d) APCM; and (e) SUBC on the Washington DC HSI.

and (b) depicts estimated abundance maps stemmed from *Bi*-472 *ICE* for two endmembers: 1) manmade material and 2) (most probably) soil/grass of class 1. Fig. 15 illustrates clustering results emerged from: (a) *k-means*; (b) *HAC*; (c) *FCM*; (d) *APCM*; 475 and (e) *SUBC* on the Washington DC *HSI* dataset. It should be highlighted that, apart from *SUBC*, all other algorithms falsely classify water and asphalt road pixels to one class. On the other hand, *SUBC* correctly distinguishes pixels that belong to the water class from all other pixels that belong to the remaining classes. 481

As it has been highlighted throughout the paper, the key idea 482 of the proposed method is to perform unmixing at its first stage, 483 in order to take the abundance representations of the pixels 484 and then, at the second stage, to perform clustering based on 485 the pixels abundance vector representations. Clearly, one could 486 choose any unmixing method in the first stage and any clustering 487 method in the second stage of the algorithm. In order to justify 488 the choice of *BiICE* in the first stage, we compare it against 489 two AE algorithms: 1) a quadratic programming (QP) technique 490 [45], which does not exploit sparsity and 2) the sparse unmix-491 ing by variable splitting and augmented Lagrangian (SUnSAL) 492 algorithm [46], which, as *BiICE*, imposes sparsity. That is, we 493 substitute BiICE with QP and SUnSAL at the first stage of the 494 proposed method. Leaned on Table VII, which depicts the OA 495

Fig. 13. (a) First PCA band; (b) 100th band of Washington DC; and (c) reference map [44].

classification map provided by [49] and used here as a referencemap.

(c)

Fig. 13 depicts: (a) first *PCA* band; (b) 100th band; and (c) reference map of a 100×100 subimage of the Washington DC mall *HSI* [44]. It should be noticed that the reference map is provided only for qualitative visualization assessment and it is not accurate for a thorough quantitative assessment. Fig. 14(a)



3. Roofs

Asphalt

Road

5. Water

Clustering results emerged from: (a) k-means, (b) HAC, (c) FCM,

(d) APCM and (e) SUBC on the Pavia center HSI.





Fig. 12.

TABLE VII COMPARATIVE RESULTS OF SU ALGORITHMS ON HSI DATASETS IN TERMS OF OA

	Synthetic	Salinas	Pavia
QP	83.67	74.32	71.20
SUnSAL BiICE	97.50 99.28	82.71 93.04	87.52 96.30

of the three cases, the QP algorithm attains the worst perfor-496 mance (since it does not take into account that by the nature of 497 the problem, the abundance vectors exhibit sparsity), whereas 498 499 SUnSAL exhibits significantly improved performance compared to QP, yet inferior, compared to BiICE, especially for real data. 500 Moreover, SUnSAL comes at the additional expense of manually 501 fine-tuning nontrivial parameters, such as a sparsity promoting 502 parameter λ . 503

The choice of APCM in the second stage of the algorithm is 504 505 justified mainly by the fact that it is able to estimate automatically the underlying number of clusters in the dataset. Moreover, 506 focusing on the first four lines of Tables I, III, and IV, the OA 507 of APCM is significantly higher from all other state of the art 508 clustering methods (note that all these algorithms are applied on 509 510 the same dataset, i.e., the spectral signature representations of the HSI pixels). 511

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IV. CONCLUSION AND FUTURE DIRECTIONS

513 The key challenge of the proposed method (SUBC) is the identification of spatially homogeneous regions comprising different 514 materials. The method consists of two main stages (unmixing 515 and clustering) and generates three significant (by)products, 516 namely: 1) endmembers; 2) abundance vectors (abundance 517 maps); and 3) clusters (classification maps). The key feature of 518 SUBC is the utilization of the abundance representations of the 519 HSI pixels (as they result from the unmixing stage) in the cluster-520 ing stage. The advantage of using the abundance representation 521 instead of the basic spectral representation of the pixels is that 522 the former, in contrast to the latter, provides subpixel level infor-523 mation, which in turn favors more detailed classification maps. 524 Moreover, the abundance representation is likely to give rise to 525 more well-discriminated clusters that live on subspaces of the 526 abundance space, due to the fact that only a few materials are 527 expected to contribute to the formation of a HSI pixel (sparsity 528 issue). As a consequence, subspace clustering algorithms could 529 also be considered as an alternative in the final stage of the algo-530 rithm, since the abundance representations are likely to lead to 531 clusters that live to subspaces of the abundance space. SUBC is 532 unsupervised and does not require class information knowledge 533 of the dataset under study. Moreover, it is image independent, 534 it alleviates the "curse of dimensionality" issue and enhances 535 localization and accuracy since it operates in the subpixel level 536 of information. However, it is noted again that the correct iden-537 tification of the endmembers number and their correspondence 538 539 to physical objects/materials is undoubtedly the most critical

step for successful SU and, as a consequence, for the clustering 540 processes. 541

Experimental results show that *SUBC* compares favorably to 542 other related methods. This gives us confidence to claim that the 543 performance of the proposed method remains consistent with 544 high-spatial resolution airborne data. It is capable of identifying 545 compact regions and spectral regions that lack training data. 546

In terms of future directions, the full potential of this al-547 gorithm will be investigated with additional hyperspectral ac-548 quisitions of higher mixture complexity. In addition, this study 549 could be reinforced and expanded in the case of existing and 550 future satellite hypespectral data imagery of lower spatial res-551 olutions where increased complexity issues for the tasks of 1) 552 endmember identification; 2) resolving shadowing effects; and 553 3) facing oblique viewing and illumination angles arise. More-554 over, subspace clustering algorithms could be utilized, since as 555 we discussed earlier, they suit nicely in the nature of the problem 556 in the abundance space. 557

ACKNOWLEDGMENT

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The AVIRIS data were provided courtesy of NASA/JPL-559 Caltech in Pasadena, CA, USA, via the EXELIS Visual In-560 formation Solutions Inc., 2012. 561

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