

A SOFT CONSTRAINED MAP ESTIMATOR FOR SUPERVISED HYPERSPECTRAL SIGNAL UNMIXING

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ABSTRACT

In this paper a novel approach is presented for spectral unmixing in hyperspectral remote sensing images. By assuming knowledge of the number and spectral signatures of the materials present in an image, efficient estimation for their corresponding fractions in the pixels of the image is developed based on a recently proposed maximum a posteriori probability (MAP) method. By exploiting the constraints naturally imposed to the problem, closed form expressions are derived for the statistical parameters required by the MAP estimator. The proposed method offers significant computational savings compared to a quadratic programming based approach. As shown by simulations conducted on real hyperspectral data collected by the HYDICE sensor, this gain in complexity is attained with only a slight degradation in performance.

1. INTRODUCTION

Hyperspectral remote sensing has gained considerable attention in recent years, due to its high number of applications [1]. Hyperspectral imaging sensors have the ability to sample the reflective region of the electromagnetic spectrum at a large number of contiguous narrow spectral bands. Thus, for every pixel in a hyperspectral image, an almost continuous radiance spectrum is created. This spectral information can be suitably exploited to determine various features of interest in a remote scene. A problem of major importance in several applications is spectral unmixing [2]. Spectral unmixing is the procedure by which the measured spectrum of a mixed pixel is decomposed into a number of constituent spectra, called endmembers, and the corresponding fractions, or abundances, that indicate the proportion of each endmember present in the pixel. Linear spectral unmixing [3], which considers that the spectrum of a mixed pixel is a linear combination of its endmembers' spectra, is more commonly used in practice.

Hyperspectral unmixing methods can be categorized into supervised and unsupervised. Supervised techniques, [4]-[6], assume that the spectral signatures of the endmembers are known a priori. On the contrary, in unsupervised methods, [7]-[8], the endmembers' spectra must be estimated from the data. In what follows, we assume that the spectral signatures of the materials present in the image are already known and consider the problem of estimating the corresponding abundances. Based on their physical interpretation, two hard constraints are imposed on the abundance fractions of the materials in a pixel; they should be nonnegative and sum to one [9]. Therefore, abundance estimation can be

viewed as a convex optimization problem [10], which can be solved numerically through computationally costly quadratic programming.

In this paper, a recently proposed soft constrained maximum a posteriori probability (MAP-s) method [11] is adopted and properly adjusted for abundance estimation in hyperspectral images. In [11], the hard constraints of the estimation problem are considered as a priori knowledge of the estimator and described via a suitably computed multivariate Gaussian distribution. The mean and covariance matrix of this distribution are obtained by solving a linear matrix inequalities (LMI) optimization problem [12]. In this work, by exploiting the symmetry of the constraints of the abundance estimation problem, closed form expressions are derived for both the mean and the covariance matrix of the multivariate Gaussian distribution. These expressions can be used directly to construct the estimator, thus avoiding the solution of an LMI optimization problem. It should be noted that due to the statistical approach followed to describe the constraints, the MAP-s estimator will violate the initial hard constraints. To be able to assess the performance of the estimator, a projection of the obtained solution in the set of constraints is also described. The proposed estimation method offers significant computational savings, compared to existing constrained optimization techniques, making it especially attractive for applications involving real time processing of hyperspectral data. As verified by simulations, this computational gain comes with no essential loss in the performance of the method.

The rest of the paper is organized as follows. In Section 2 the abundance estimation problem is defined. The proposed MAP-s estimator is described in Section 3. Some simulation results are provided in Section 4, and concluding remarks are given in Section 5.

2. PROBLEM FORMULATION

In a hyperspectral image, each pixel is assigned an L -dimensional vector \mathbf{r} , where L is the number of spectral bands. The elements of \mathbf{r} correspond to the reflectance energy measured at the respective spectral bands. By assuming that there exist p distinct materials in the image scene, also called endmembers, we define the $L \times p$ matrix $\mathbf{C} = [\mathbf{c}_1 \mathbf{c}_2 \dots \mathbf{c}_p]$, where \mathbf{c}_j is the spectral signature vector of the j th material. Let $\mathbf{x} = (x_1, x_2, \dots, x_p)^T$ be the $p \times 1$ vector of abundances associated with \mathbf{r} , i.e. x_j is the abundance fraction of the j th material in the pixel \mathbf{r} . A commonly used model to describe the combination of materials in a pixel, is

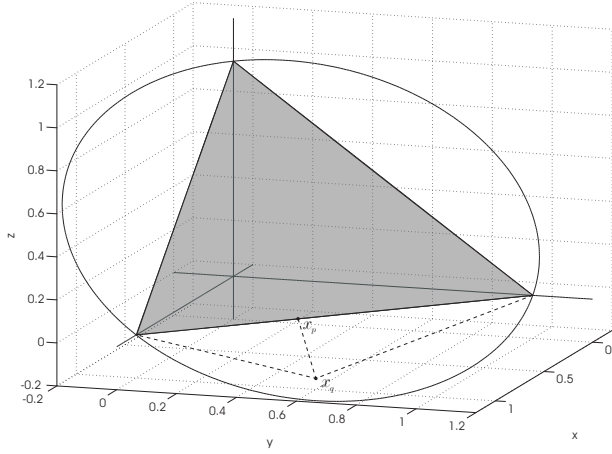


Figure 1: ASC and ANC define a 2-simplex in the three-dimensional space.

the so-called linear mixing model (LMM) [3]. According to this model, \mathbf{r} is expressed as follows:

$$\mathbf{r} = \mathbf{C}\mathbf{x} + \mathbf{v}, \quad (1)$$

where \mathbf{v} is the measurement noise assumed to be zero-mean and with covariance Σ_v . Assuming that the spectral signatures $\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_p$ of the endmembers are already known, we are interested in estimating the vector \mathbf{x} of abundances. Two constraints are naturally imposed on the abundance vector \mathbf{x} . The abundance sum-to-one constraint (ASC), i.e.,

$$\sum_{i=1}^p x_i = 1, \quad (2)$$

and the abundance non-negativity constraint (ANC), i.e.,

$$0 \leq x_i \leq 1, \quad i = 1, 2, \dots, p. \quad (3)$$

By viewing \mathbf{x} as a point in a p -dimensional space, it is easily shown that the above constraints define a standard $(p-1)$ -simplex [13], i.e. a simplex whose vertices are the points corresponding to the columns of the identity matrix. By denoting this simplex by \mathbb{S} , each point \mathbf{x} associated with an image pixel \mathbf{r} must reside inside the hypervolume of \mathbb{S} . A pictorial representation of the ANC and ASC in the three-dimensional space is provided in Fig. 1. In this case, all points must lie on the surface area of the standard 2-simplex, which corresponds to the shaded area in the figure.

3. THE PROPOSED METHOD

The problem defined in the previous section can be dealt with as a least squares (LS) minimization problem with constraints. This turns out to be a convex optimization problem [10], whose solution relies on quadratic programming methods. Applying such a method may become prohibitive, due to its high computational complexity. In this paper we follow an alternative approach, by properly modifying and extending the recently proposed soft-constrained maximum a posteriori (MAP-s) estimator of [11]. The MAP-s estimator belongs to the class of superefficient estimators, i.e. it always provides better performance than the LS estimator, in terms of the matrix mean square error (MSE). Let $\Sigma_{LS} \triangleq (\mathbf{C}^T \Sigma_v^{-1} \mathbf{C})^{-1}$ denote the covariance matrix of the unconstrained LS estimator.

An estimator $\hat{\mathbf{x}}$ is said superefficient or LS-dominating if its MSE does not exceed the MSE of the LS estimator, i.e.

$$E[(\mathbf{x} - \hat{\mathbf{x}})(\mathbf{x} - \hat{\mathbf{x}})^T] \leq \Sigma_{LS}. \quad (4)$$

To provide MSE improvement, superefficient estimators exploit some a priori knowledge about the parameters to be estimated. In the problem under consideration, the a priori knowledge is the set of constraints which are naturally imposed on \mathbf{x} . Under the assumption that \mathbf{x} is a random vector with prior Gaussian distribution¹, the MAP-s estimate of \mathbf{x} is:

$$\hat{\mathbf{x}} = (\mathbf{C}^T \Sigma_v^{-1} \mathbf{C} + \bar{\Sigma}^{-1})^{-1} (\mathbf{C}^T \Sigma_v^{-1} \mathbf{r} + \bar{\Sigma}^{-1} \bar{\mathbf{x}}), \quad (5)$$

where $\bar{\mathbf{x}} \in \mathbb{R}^p$ and $\bar{\Sigma} \in \mathbb{R}^{p \times p}$ are the mean and covariance matrix of \mathbf{x} , respectively. The main idea here, is to select the parameters $\bar{\mathbf{x}}$ and $\bar{\Sigma}$, based on the knowledge of the polytope of constraints \mathbb{S} , so as to guarantee the LS-domination property (4), $\forall \mathbf{x} \in \mathbb{S}$. After some calculations reported in [11], the LS-domination condition (4) can be rewritten in terms of $\bar{\Sigma}$ and $\bar{\mathbf{x}}$, as follows:

$$\bar{\Sigma} \geq \frac{1}{2} [(\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^T - \Sigma_{LS}]. \quad (6)$$

In order to compute the most appropriate parameters $\bar{\mathbf{x}}$ and $\bar{\Sigma}$, according to the constraint set \mathbb{S} , Lemma 1 of [11] proved for positive definite matrices needs to be extended for positive semidefinite matrices. This is so because in the problem under consideration the polytope of constraints \mathbb{S} lies on a hyperplane of dimension $(p-1)$ in the p -dimensional space.

Lemma 3.1. *Let $\mathbf{P} = \mathbf{P}^T \geq \mathbf{0}$ and $\mathbf{x} \in R(\mathbf{P})$, where $R(\cdot)$ denotes column space. Then if*

$$\mathbf{P} \geq \mathbf{x}\mathbf{x}^T \iff \mathbf{x}^T \mathbf{P}^\dagger \mathbf{x} \leq 1, \quad (7)$$

where $(\cdot)^\dagger$ denotes the Moore-Penrose pseudoinverse.

Proof. It follows directly from the properties of the generalized Schur complement [15]. According to the Albert nonnegative conditions [15], for matrices \mathbf{P} , \mathbf{C} and \mathbf{B} with appropriate dimensions, the following two statements are equivalent:

i) $\mathbf{P} \geq \mathbf{0}$ and $\mathbf{C} - \mathbf{B}^T \mathbf{P}^\dagger \mathbf{B} \geq \mathbf{0}$ and $R(\mathbf{B}) \subset R(\mathbf{P})$

ii) $\mathbf{C} \geq \mathbf{0}$ and $\mathbf{P} - \mathbf{B}\mathbf{C}^\dagger \mathbf{B}^T \geq \mathbf{0}$ and $R(\mathbf{B}^T) \subset R(\mathbf{C})$.

Therefore, if $\mathbf{P} \geq \mathbf{0}$, $\mathbf{C} \geq \mathbf{0}$, $R(\mathbf{B}) \subset R(\mathbf{P})$, and $R(\mathbf{B}^T) \subset R(\mathbf{C})$, then

$$\mathbf{P} \geq \mathbf{B}\mathbf{C}^\dagger \mathbf{B}^T \iff \mathbf{C} \geq \mathbf{B}^T \mathbf{P}^\dagger \mathbf{B}.$$

Setting $\mathbf{B} = \mathbf{x}$ and $\mathbf{C} = \mathbf{I}$ completes the proof. \square

Let $\varepsilon(\mathbf{c}, \mathbf{P}) \triangleq \{\mathbf{x} : (\mathbf{x} - \mathbf{c})^T \mathbf{P}^\dagger (\mathbf{x} - \mathbf{c}) \leq 1\}$ denote an ellipsoid of center \mathbf{c} and \mathbf{P} is a symmetric positive semidefinite matrix. Lemma 3.1 suggests that matrix $(\mathbf{P} - \mathbf{x}\mathbf{x}^T)$ is positive semidefinite if and only if every point \mathbf{x} belongs to the ellipsoid $\varepsilon(\mathbf{0}, \mathbf{P})$. By setting

$$\mathbf{P} \triangleq 2\bar{\Sigma} + \Sigma_{LS}, \quad (8)$$

¹A different prior distribution for \mathbf{x} could also be adopted, leading to a different estimation approach [14].

Lemma 3.1 provides a geometrical interpretation of Eq. (6): an MSE improvement over the LS estimator is achieved if and only if the ellipsoid $\varepsilon(\bar{\mathbf{x}}, \mathbf{P})$ contains the polytope of constraints \mathbb{S} .

Capitalizing on this result, it can be shown, as in [11], that $\bar{\Sigma}$ and $\bar{\mathbf{x}}$ must satisfy the following set of linear matrix inequalities (LMI):

$$\begin{bmatrix} 2\bar{\Sigma} + \bar{\Sigma}_{LS} & \mathbf{e}_i - \bar{\mathbf{x}} \\ (\mathbf{e}_i - \bar{\mathbf{x}})^T & 1 \end{bmatrix} \geq 0 \quad i = 1, 2, \dots, p \quad (9)$$

$$\bar{\Sigma} \geq 0,$$

where \mathbf{e}_i , $i = 1, 2, \dots, p$ are the vertices of the $(p-1)$ -simplex, which coincide with the columns of the identity matrix. The MAP-s estimator can then be summarized as follows: given \mathbb{S} and Σ_{LS} select the parameters $\bar{\mathbf{x}}$ and $\bar{\Sigma}$ so that:

$$\min_{\bar{\mathbf{x}}, \bar{\Sigma}} \det(\bar{\Sigma}) \text{ subject to (9),} \quad (10)$$

where $\det(\cdot)$ denotes the determinant of a matrix.

In geometrical terms, minimization of the determinant of $\bar{\Sigma}$ corresponds to finding the minimum volume ellipsoid containing \mathbb{S} . The above minimization criterion does not guarantee the minimum achievable MSE, but gives rise to standard convex LMI problems that can be solved in polynomial time [12]. Although the minimization process is based on both the parameters $\bar{\mathbf{x}}$ and $\bar{\Sigma}$, it has been shown that for symmetric constraints the optimal solution is obtained when $\bar{\mathbf{x}}$ is selected as the center of symmetry of the constraint set.

In the problem of estimating the abundance vectors in a hyperspectral image, the polytope of constraints is explicitly defined as a standard $(p-1)$ -simplex \mathbb{S} . It can be shown that the minimum volume ellipsoid circumscribing \mathbb{S} is the hypersphere $\varepsilon(\bar{\mathbf{x}}, \mathbf{P})$, which is defined by

$$\mathbf{P}^\dagger = \begin{bmatrix} 1 & -\frac{1}{p-1} & \dots & -\frac{1}{p-1} \\ -\frac{1}{p-1} & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\frac{1}{p-1} \\ -\frac{1}{p-1} & \dots & -\frac{1}{p-1} & 1 \end{bmatrix}, \quad (11)$$

while

$$\bar{\mathbf{x}} = [1/p, 1/p, \dots, 1/p]^T, \quad (12)$$

is selected as the center of the $(p-1)$ -dimensional simplex. For instance, for $p = 3$ the minimum volume ellipsoid $\varepsilon(\bar{\mathbf{x}}, \mathbf{P})$ reduces to the disc shown in Fig. 1. Matrix \mathbf{P} , whose Moore-Penrose pseudoinverse is given by (11), is a singular symmetric positive semidefinite matrix of rank $p-1$ expressed as follows

$$\mathbf{P} = \begin{bmatrix} \frac{(p-1)^2}{p^2} & -\frac{p-1}{p^2} & \dots & -\frac{p-1}{p^2} \\ -\frac{p-1}{p^2} & \frac{(p-1)^2}{p^2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\frac{p-1}{p^2} \\ -\frac{p-1}{p^2} & \dots & -\frac{p-1}{p^2} & \frac{(p-1)^2}{p^2} \end{bmatrix} \quad (13)$$

It should be noted that since \mathbf{x} satisfies the constraint (2) and the elements of each row of \mathbf{P} add to zero, $\mathbf{x} - \bar{\mathbf{x}} \in R(\mathbf{P})$, as required by the assumptions of Lemma 3.1.



Figure 2: Urban HYDICE hyperspectral dataset, band 80.

From (8), (13) and assuming knowledge of Σ_{LS} , $\bar{\Sigma}$ can be written as follows:

$$\bar{\Sigma} = \frac{1}{2}(\mathbf{P} - \Sigma_{LS}) \quad (14)$$

By substituting $\bar{\mathbf{x}}$ and $\bar{\Sigma}$ from (12) and (14) in (5), an estimate of the abundance vector is directly obtained. These quantities need to be computed only once and are then used for the estimation of the abundance vector of each pixel in the image. It should be noted that due to the form of matrix \mathbf{P} , $\bar{\Sigma}$ given by (14) is near to singular. This may seriously affect the estimate in (5), where the inverse of $\bar{\Sigma}$ need to be computed. To tackle this problem, some kind of regularization can be applied, i.e., the inverse of $\bar{\Sigma}$ is computed as $(\bar{\Sigma} + \delta \mathbf{I})^{-1}$, where δ is a small positive constant and \mathbf{I} is the $p \times p$ identity matrix.

3.1 Imposing the hard constraints

As described above, the MAP-s estimator assumes that the vector of abundances has a prior Gaussian distribution, i.e. $\mathbf{x} \sim N(\bar{\mathbf{x}}, \bar{\Sigma})$, where $\bar{\mathbf{x}}$, $\bar{\Sigma}$ are given by (12) and (14) respectively. Due to this statistical assumption, for some pixels in the image, the corresponding abundance vectors may lie outside the polytope \mathbb{S} , violating the hard constraint (3). However, as it will become clear in the next section, in order to assess the performance of the proposed method for hyperspectral images, the hard constraints must be somehow imposed to the estimator. Let \mathbf{x}_q be an estimated vector violating (3). The main idea is to replace \mathbf{x}_q with a new estimation point, by means of projecting \mathbf{x}_q on the polytope \mathbb{S} . In this way, the projection point will be the closest point to \mathbf{x}_q satisfying the constraints of the problem. Unfortunately, there is no known closed form expression for the projection of a point on the standard $(p-1)$ -simplex in the p -dimensional space. In the following we propose an approximate solution, which is based on the Euclidean distances of \mathbf{x}_q from the vertices of \mathbb{S} . Since the polytope \mathbb{S} is convex, any point \mathbf{x}_p on a $(p-1)$ -dimensional hypersurface of \mathbb{S} can be expressed as a linear combination of the corresponding $p-1$ vertices of the polytope, i.e.

$$\mathbf{x}_p = \theta_1 \mathbf{e}_1 + \theta_2 \mathbf{e}_2 + \dots + \theta_{p-1} \mathbf{e}_{p-1}, \quad (15)$$

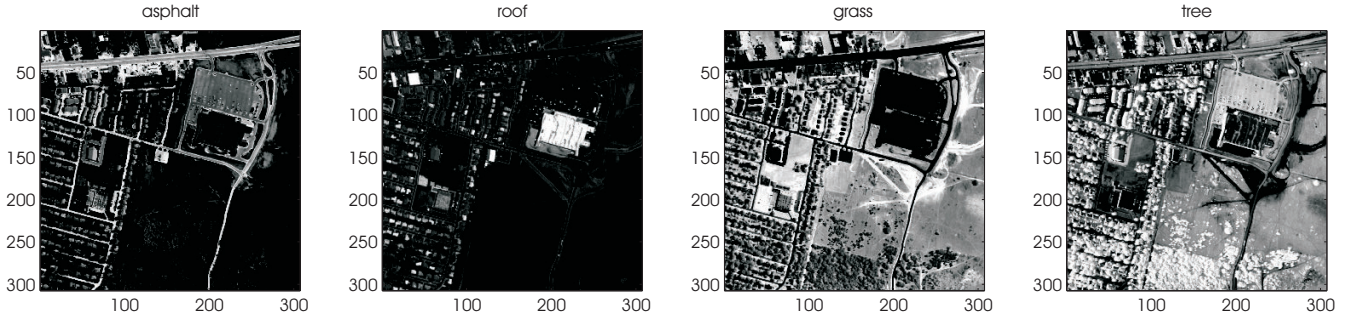


Figure 3: Abundance estimation using quadratic programming techniques

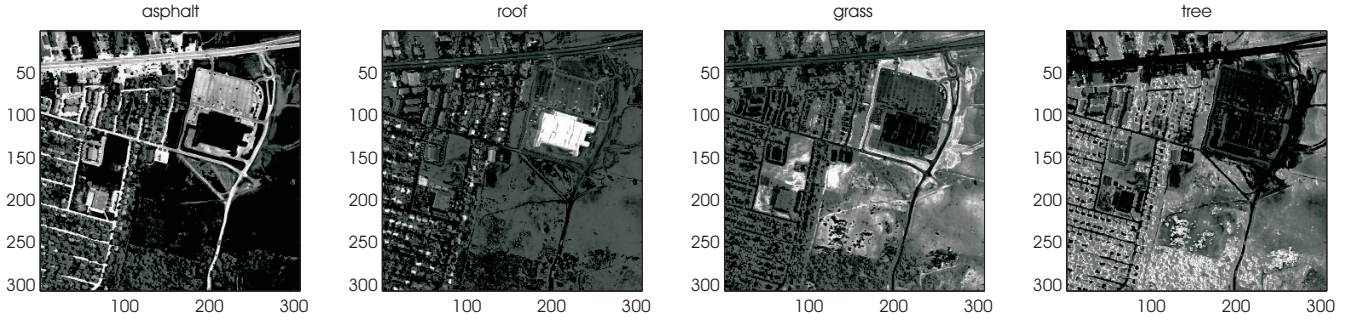


Figure 4: Abundance estimation using the MAP-s estimator and solving the LMI optimization problem

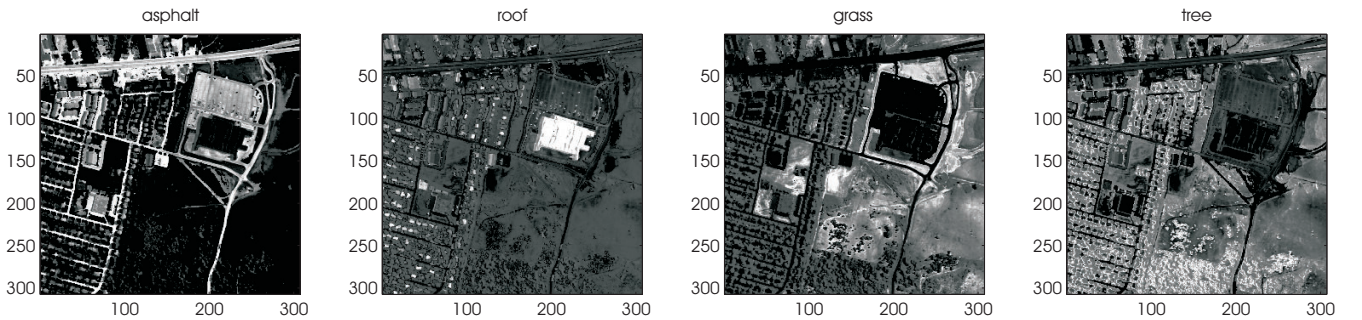


Figure 5: Abundance estimation using the closed form expression of the MAP-s estimator

where θ_i are weight coefficients such that $\sum_{i=1}^{p-1} \theta_i = 1$ and $\theta_i \geq 0$, $i = 1, 2, \dots, p-1$. Apparently, the vertex excluded in (15) is the one with the largest Euclidean distance from \mathbf{x}_q , which without loss of generality is assumed to be \mathbf{e}_p . Let d_1, d_2, \dots, d_{p-1} denote the Euclidean distances between \mathbf{x}_q and the $p-1$ remaining vertices of the polytope. Then, the weight coefficients θ_i in (15) can be computed according to the following relation:

$$\theta_i = \frac{\varphi(d_i)}{\sum_{j=1}^{p-1} \varphi(d_j)}, \quad i = 1, 2, \dots, p-1, \quad (16)$$

where $\varphi(\cdot)$ is a properly selected function. Two possible choices are $\varphi(x) = 1/x$ and $\varphi(x) = e^{1/x}$. As can be easily verified, in both cases the weight parameter θ_i is reversely proportional to the Euclidean distance d_i , with the second choice weighting more heavily closely located vertices.

4. SIMULATIONS

In this section, we use real hyperspectral data to evaluate the performance of the proposed modified MAP-s estimator, when compared to the constrained quadratic programming approach. The data correspond to an urban image scene, shown in Fig. 2, and have been collected by the Hyperspectral Digital Imagery Collection Experiment (HYDICE) sensor. The sensor works in 210 spectral bands, in the region from 400 to 2500nm, with a spectral resolution of 10nm. After removing the low SNR bands, 162 spectral bands remain available, i.e. $L=162$. Four endmembers are present in the image, namely asphalt, roof, grass and tree. The spectral signatures of these endmembers have been identified using a supervised technique, [9], i.e. areas in the image which seem to contain a pure material are used to extract the spectrum of this material.

So far, it has been assumed that the noise covariance matrix Σ_v is known. Note that Σ_{LS} used in (14) to compute the covariance matrix $\bar{\Sigma}$, depends on Σ_v . As a result, estimation

of the noise covariance matrix of the image is a necessary preprocessing step of the proposed algorithm, which may affect the overall performance of the estimator. In our simulation experiments, Σ_v has been computed using the shift-difference method, as in [16].

In Figs. 3, 4 and 5, the results of three abundance estimation methods are depicted. Each figure comprises four images corresponding to the four endmembers under consideration. A pure black pixel in an image indicates that the abundance of the respective endmember is zero, while a pure white pixel represents an abundance value equal to one. All other abundance values between zero and one are illustrated according to the different tones of gray. In Fig. 3, a quadratic programming based technique has been applied to estimate the abundances. In Figs. 4 and 5, the MAP-s estimator has been implemented either by solving an LMI problem or by using directly the closed form expressions derived in this paper, respectively. We observe that the proposed method succeeds in discriminating all four endmembers with sufficiently high accuracy. Its performance is similar to that of the LMI-based approach, as shown by comparing Figs. 4 and 5. Compared to the convex optimization based method, there is some degradation in performance, even though the asphalt endmember seems to be better resolved using the MAP-s method. Recall, however, that the computational complexity of the proposed method is much lower, compared to the one required to numerically solve a convex optimization problem for each pixel in the hyperspectral image.

5. CONCLUSION

This paper has addressed the problem of abundance estimation in hyperspectral signal unmixing, subject to full additivity and nonnegativity constraints. Instead of solving numerically this convex optimization problem, we have followed a novel approach stemming from a recently reported MAP estimation method. The proposed algorithm has almost similar performance to the much more computationally demanding numerical method, thus making it especially attractive for real time processing of hyperspectral data.

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