LINEAR MIXTURE MODELS AND PARTIAL UNMIXING IN MULTI- AND HYPERSPECTRAL IMAGE DATA

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ABSTRACT: As a supplement or an alternative to classification of hyperspectral image data the linear mixture model is considered in order to obtain estimates of abundance of each class or end-member in pixels with mixed membership. Full unmixing and the partial unmixing methods orthogonal subspace projection (OSP), constrained energy minimization (CEM) and an eigenvalue formulation alternative are dealt with. The solution to the eigenvalue formulation alternative proves to be identical to the CEM solution. The matrix inversion involved in CEM can be avoided by working on (a subset of) orthogonally transformed data such as signal maximum autocorrelation factors, MAFs, or signal minimum noise fractions, MNFs. This will also cause the noise isolated in the MAF/MNFs not included in the analysis not to influence the partial unmixing result. CEM and the eigenvalue formulation alternative enable us to perform partial unmixing when we know the desired end-member spectra only and not the full set of end-member spectra. This is an advantage over full unmixing and OSP. An example with a simple simulated 2-band image shows the ability of the CEM method to isolate the desired signal. A case study with a 30 bands subset of AVIRIS data from the Mojave Desert, California, USA, indicates the utility of CEM to more realistic data.

KEY WORDS: matched filtering; orthogonal subspace projection, OSP; constrained energy minimization, CEM; generalized eigenvalue problem

1 INTRODUCTION

In ordinary discriminant analysis which is often used to classify for instance multi- or hyperspectral remote sensing image data it is assumed that each observation (or pixel) is a member of one and only one of a number of pre-determined classes. Linear mixture models allow us to estimate the abundance of each class in pixels with mixed class membership, [10, 8, 17].

2 LINEAR MIXING

We assume that the signal measured at each pixel consists of a linear combination of p so-called end-members. End-members are pure pre-determined classes with 100% abundance of one element and with no mixtures. We think of our l-dimensional signal for end-member i as a vector $\boldsymbol{m}_i = [m_{i1} \ \ldots \ m_{il}]^T, \ i = 1, \ldots, p$ and represent the end-members by a matrix

$$\boldsymbol{M} \ = \ [\boldsymbol{m}_1 \ \ldots \ \boldsymbol{m}_p] \ = \ \begin{bmatrix} m_{11} & \cdots & m_{p1} \\ \vdots & \ddots & \vdots \\ m_{1l} & \cdots & m_{pl} \end{bmatrix} \tag{1}$$

with one column for each end-member. We write each observation $\boldsymbol{r}(x,y) = [r_1(x,y)\ \ldots\ r_l(x,y)]^T$ as a linear combination of the end-members $\boldsymbol{M}$; the abundances $\boldsymbol{\alpha}(x,y) = [\alpha_1(x,y)\ \ldots\ \alpha_p(x,y)]^T$ are the coefficients

$$\boldsymbol{r}(x,y) \;=\; \boldsymbol{M}\boldsymbol{\alpha}(x,y) + \boldsymbol{n}(x,y) \tag{2}$$

where $\boldsymbol{n}(x,y) = [n_1(x,y)\ \ldots\ n_l(x,y)]^T$ is the residual or the noise, i.e. the variation in $\boldsymbol{r}(x,y)$ not explained by the model. This is the linear mixture model. The term linear means linear in the coefficients. The expected value of the noise $\mathrm{E}\{\boldsymbol{n}\} = \boldsymbol{0}$. In linear models a constant term α_0 (from now on we omit (x,y) from the notation) is often introduced. Here, α_0 represents effects not explained by the chosen end-members. If we introduce α_0 we get

$$\boldsymbol{M} \;=\; \begin{bmatrix} 1 & m_{11} & \cdots & m_{p1} \\ 1 & \vdots & \ddots & \vdots \\ 1 & m_{1l} & \cdots & m_{pl} \end{bmatrix} \quad \text{and} \quad \boldsymbol{\alpha} \;=\; [\alpha_0\ \alpha_1\ \ldots\ \alpha_p]^T. \tag{3}$$

Sometimes the column of ones is replaced by a column of zeros. This represents the end-member "total shade."

To solve the system of equations involved we minimize the sum of squared residuals $\boldsymbol{n}^T\boldsymbol{n}$ or more generally $\boldsymbol{n}^T\boldsymbol{\Sigma}_n^{-1}\boldsymbol{n}$ where $\boldsymbol{\Sigma}_n$ is the dispersion or covariance matrix of the residuals. This is done by setting the partial derivative $\partial(\boldsymbol{n}^T\boldsymbol{\Sigma}_n^{-1}\boldsymbol{n})/\partial\boldsymbol{\alpha} = \boldsymbol{0}$. The result is

$$\boldsymbol{\alpha} \;=\; (\boldsymbol{M}^T\boldsymbol{\Sigma}_n^{-1}\boldsymbol{M})^{-1}\boldsymbol{M}^T\boldsymbol{\Sigma}_n^{-1}\boldsymbol{r}. \tag{4}$$

The estimator $\boldsymbol{\alpha}$ is central with dispersion $(\boldsymbol{M}^T\boldsymbol{\Sigma}_n^{-1}\boldsymbol{M})^{-1}$. When $\boldsymbol{\Sigma}_n = \sigma^2\boldsymbol{I}$ where $\boldsymbol{I}$ is the $l \times l$ unit matrix and σ^2 is the variance of all residuals, $\mathrm{V}\{n_i\} = \sigma^2$

$$\boldsymbol{\alpha} \;=\; (\boldsymbol{M}^T\boldsymbol{M})^{-1}\boldsymbol{M}^T\boldsymbol{r} \tag{5}$$

with dispersion $\sigma^2(\boldsymbol{M}^T\boldsymbol{M})^{-1}$.

To evaluate the goodness of the model we use $R^2 = (\tilde{\boldsymbol{r}}^T\tilde{\boldsymbol{r}} - \boldsymbol{n}^T\boldsymbol{\Sigma}_n^{-1}\boldsymbol{n})/\tilde{\boldsymbol{r}}^T\tilde{\boldsymbol{r}}$, the coefficient of determination (if $\boldsymbol{M}$ contains the column of ones $\tilde{\boldsymbol{r}}$ is $\boldsymbol{r}$ centered, if not $\tilde{\boldsymbol{r}} = \boldsymbol{r}$), and the estimate of residual variance, $s^2 = (\boldsymbol{n}^T\boldsymbol{\Sigma}_n^{-1}\boldsymbol{n})/(l-p-1)$. s is called the root mean square error, RMSE. $l-p-1$, the degree of freedom, must be positive. If an extra column is added to $\boldsymbol{M}$ p is replaced by $p+1$.

3 PARTIAL UNMIXING

To perform a full unmixing one needs to know the spectra for all end-members present in the scene. This knowledge is often not available. Therefor partial unmixing methods where we estimate the presence of one or a few desired spectra only are important.

Partial unmixing builds on the usual linear mixture model in equation 2. We split the $\boldsymbol{M}\boldsymbol{\alpha}$ term into two terms, one which is the desired end-member $\boldsymbol{d}$ with a corresponding abundance α_p (without loss of generality we place $\boldsymbol{d}$ in the last column of $\boldsymbol{M}$), and one which consists of the undesired end-members $\boldsymbol{U}$ with a corresponding $(p-1) \times 1$ vector, $\boldsymbol{\gamma}$, of abundances. $\boldsymbol{U}$ contains the first $p-1$ columns of $\boldsymbol{M}$ and $\boldsymbol{\gamma}$ contains the first $p-1$ elements of $\boldsymbol{\alpha}$. Hence

$$\boldsymbol{r} \;=\; \boldsymbol{M}\boldsymbol{\alpha} + \boldsymbol{n} \;=\; \boldsymbol{d}\alpha_p + \boldsymbol{U}\boldsymbol{\gamma} + \boldsymbol{n}. \tag{6}$$

$\boldsymbol{U}\boldsymbol{\gamma}$ is often termed the interference. In partial unmixing we want to develop methods to eliminate or minimize the effect of $\boldsymbol{U}$ and $\boldsymbol{\gamma}$. Often the term matched filtering is applied to such methods.

3.1 Orthogonal Subspace Projection, OSP

The idea in OSP, [11, 6], is to project $\boldsymbol{r}$ onto a subspace where $\boldsymbol{\gamma}$ is removed from the linear mixture model, equation 6. Applying the $l \times l$ matrix $\boldsymbol{P} = \boldsymbol{I} - \boldsymbol{U}(\boldsymbol{U}^T\boldsymbol{U})^{-1}\boldsymbol{U}^T$ we obtain

$$\boldsymbol{P}\boldsymbol{r} \;=\; \boldsymbol{P}\boldsymbol{d}\alpha_p + \boldsymbol{U}\boldsymbol{\gamma} - \boldsymbol{U}(\boldsymbol{U}^T\boldsymbol{U})^{-1}\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{\gamma} + \boldsymbol{P}\boldsymbol{n} \;=\; \boldsymbol{P}\boldsymbol{d}\alpha_p + \boldsymbol{P}\boldsymbol{n}. \tag{7}$$

We have indeed removed $\boldsymbol{\gamma}$ from the linear mixture model but as with full unmixing we need $\boldsymbol{U}$, i.e. we need all the end-member spectra, both desired and undesired.

In [16] it is shown that full linear unmixing and OSP as described in [6] are identical (except that OSP is computationally slightly more expensive).

3.2 Constrained Energy Minimization, CEM

Constrained energy minimization, CEM, [15, 18], builds on the linear mixture model in equation 6. In CEM we project $\boldsymbol{r}$ onto $\boldsymbol{w}$ with the intent to highlight presence of the desired end-member, and to suppress the presence of the undesired end-members and noise. We do this by requesting the following

1. we want the output (the projected value) to be one when we project the desired spectrum, $\boldsymbol{d}$, i.e. we want $\boldsymbol{w}^T\boldsymbol{d} = 1$;
2. in general, we want the output to be close to zero, we want its expected value to be 0, $\mathrm{E}\{\boldsymbol{w}^T\boldsymbol{r}\} = 0$;
3. also we want to minimize the expected value of the squared difference between the output, $\boldsymbol{w}^T\boldsymbol{r}$, and the desired output, 0, i.e. we want to minimize $\mathrm{E}\{(\boldsymbol{w}^T\boldsymbol{r} - 0)^2\}$.

Since $\mathrm{E}\{\boldsymbol{w}^T\boldsymbol{r}\} = 0$ we get $\mathrm{E}\{(\boldsymbol{w}^T\boldsymbol{r} - 0)^2\} = \mathrm{V}\{\boldsymbol{w}^T\boldsymbol{r}\}$. Hence the job is to minimize $\mathrm{V}\{\boldsymbol{w}^T\boldsymbol{r}\} = \boldsymbol{w}^T\boldsymbol{\Sigma}\boldsymbol{w}$ with the constraint $\boldsymbol{w}^T\boldsymbol{d} = 1$. $\boldsymbol{\Sigma}$ is the dispersion matrix of $\boldsymbol{r}$. To do this we introduce a Lagrange multiplier -2λ and minimize $F = \boldsymbol{w}^T\boldsymbol{\Sigma}\boldsymbol{w} + 2\lambda(\boldsymbol{w}^T\boldsymbol{d} - 1)$ without constraints. This is done by setting the partial derivatives $\partial F/\partial \boldsymbol{w} = \boldsymbol{0}$ and $\partial F/\partial\lambda = 0$. This leads to

$$\begin{bmatrix} \boldsymbol{\Sigma} & \boldsymbol{d} \\ \boldsymbol{d}^T & 0 \end{bmatrix}\begin{bmatrix} \boldsymbol{w} \\ \lambda \end{bmatrix} \;=\; \begin{bmatrix} \boldsymbol{0} \\ 1 \end{bmatrix} \quad \text{or} \quad \boldsymbol{w} \;=\; \frac{\boldsymbol{\Sigma}^{-1}\boldsymbol{d}}{\boldsymbol{d}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{d}} \tag{8}$$

with $\lambda = -1/\boldsymbol{d}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{d}$ (which is constant). $(\boldsymbol{w}^T\boldsymbol{r})^2$ the expectation of which is minimized is often termed "energy," hence the name CEM.

For hyperspectral data these operations will often be performed on a subset of orthogonally transformed data such as signal maximum autocorrelation factors, MAFs, or signal minimum noise fractions, MNFs, [19, 5, 1, 9, 12, 13]. In this case matrix inversion is not needed since $\boldsymbol{\Sigma}_M = \boldsymbol{I}$. Hence $\boldsymbol{w}_M = \boldsymbol{d}_M/\boldsymbol{d}_M^T\boldsymbol{d}_M$ where the subscript M denotes dispersion, projection vector and desired spectrum after the MAF or MNF transformation.

Note that nothing in the above ensures the ideal: $0 \leq \boldsymbol{w}^T\boldsymbol{r} \leq 1$. On the contrary, we have requested that $\mathrm{E}\{\boldsymbol{w}^T\boldsymbol{r}\} = 0$ which means that some projections must necessarily be negative.

As opposed to OSP and full linear unmixing, CEM does not require knowledge of all end-member spectra. Only the desired spectrum is needed.

3.3 An Eigenvalue Formulation Alternative to CEM

As a new alternative approach to CEM consider equation 6 and the projection $\boldsymbol{w}^T\boldsymbol{r}$ again

$$\boldsymbol{w}^T\boldsymbol{r} \;=\; \boldsymbol{w}^T\boldsymbol{d}\alpha_p + \boldsymbol{w}^T\boldsymbol{U}\boldsymbol{\gamma} + \boldsymbol{w}^T\boldsymbol{n}. \tag{9}$$

Consider the variance of $\boldsymbol{w}^T\boldsymbol{r}$

$$\mathrm{V}\{\boldsymbol{w}^T\boldsymbol{r}\} = \mathrm{V}\{\boldsymbol{w}^T\boldsymbol{d}\alpha_p\} + \mathrm{V}\{\boldsymbol{w}^T\boldsymbol{U}\boldsymbol{\gamma}\} + \mathrm{V}\{\boldsymbol{w}^T\boldsymbol{n}\} + 2\mathrm{Cov}\{\boldsymbol{w}^T\boldsymbol{d}\alpha_p, \boldsymbol{w}^T\boldsymbol{U}\boldsymbol{\gamma}\} \quad (10)$$

where we assume no covariation between the abundance of the desired spectrum and noise, and the abundances of the undesired spectra and noise. This can be written as

$$\begin{aligned}\boldsymbol{w}^T\boldsymbol{\Sigma}\boldsymbol{w} &= \mathrm{V}\{\alpha_p\}\boldsymbol{w}^T\boldsymbol{d}\boldsymbol{d}^T\boldsymbol{w} + \boldsymbol{w}^T\boldsymbol{U}\ \mathrm{D}\{\boldsymbol{\gamma}\}\boldsymbol{U}^T\boldsymbol{w} + \boldsymbol{w}^T\boldsymbol{\Sigma}_n\boldsymbol{w} + 2\boldsymbol{w}^T\boldsymbol{d}\ \mathrm{Cov}\{\alpha_p, \boldsymbol{\gamma}\}\boldsymbol{U}^T\boldsymbol{w} \\ &= \mathrm{V}\{\alpha_p\}\boldsymbol{w}^T\boldsymbol{d}\boldsymbol{d}^T\boldsymbol{w} + \boldsymbol{w}^T\boldsymbol{E}\boldsymbol{w} \quad (11)\end{aligned}$$

where $\boldsymbol{E}$ represents all undesired effects, namely dispersions of interference and noise, and covariance between abundances of desired and undesired spectra. $\boldsymbol{E}$ is unknown. From this we get

$$1 = \mathrm{V}\{\alpha_p\}\frac{\boldsymbol{w}^T\boldsymbol{d}\boldsymbol{d}^T\boldsymbol{w}}{\boldsymbol{w}^T\boldsymbol{\Sigma}\boldsymbol{w}} + \frac{\boldsymbol{w}^T\boldsymbol{E}\boldsymbol{w}}{\boldsymbol{w}^T\boldsymbol{\Sigma}\boldsymbol{w}}. \quad (12)$$

To minimize all the undesired effects we must minimize the last term on the right-hand-side of equation 12 and therefor since the sum is constant we must maximize the Rayleigh coefficient in the first term. Since $\boldsymbol{d}\boldsymbol{d}^T$ has rank 1 we get one solution only namely the $\boldsymbol{w}$ that satisfies the generalized eigenvalue problem

$$\boldsymbol{d}\boldsymbol{d}^T\boldsymbol{w} = \rho\boldsymbol{\Sigma}\boldsymbol{w}. \quad (13)$$

If we insert the solution for $\boldsymbol{d}$ found in equation 8 we see that these two solutions are identical with $\rho = -1/\lambda$.

4 COMPUTER PROGRAMS

Four computer programs developed at IMM are useful in this type of analysis, `unmix`, `maf`, `project`, `seed`. `unmix` performs full unmixing either without constraints or with the natural constraints that the non-negative abundances sum to one. The former problem is solved by LINPACK routines, [2], the latter by a linearly constrained least squares algorithm, LSSOL, which solves the problem: minimize $\frac{1}{2}||\boldsymbol{r} - \boldsymbol{M}\boldsymbol{\alpha}||^2$ over $\boldsymbol{\alpha}$ in this case with $\mathbf{1}^T\boldsymbol{\alpha} = 1$ and $\alpha_i \geq 0$, [4]. `maf` finds principal components, (rotated) principal factors, maximum autocorrelation factors, minimum noise fractions, canonical discriminant functions, (multiset) canonical variates and linear combinations that give maximal multivariate differences of two sets of variables, [13]. The eigenvalue problems associated with the analysis are solved by means of LAPACK routines, [3]. For a fuller description, see [12]. `project` projects data in feature space onto a unit vector representing a desired end-member spectrum. `seed` grows a training area from one or a few pixels by requesting spatial as well as spectral closeness. Spatial closeness is ensured by requesting 8-neighbor connectivity. Spectral closeness is ensured by requesting low Euclidean or Mahalanobis distance in feature space. For a fuller description, see [14].

5 CASE STUDIES

5.1 Simple, Generated Data

The data used consist of two bands, one with a centered horizontal bar and one with a centered vertical bar. The bars and the backgrounds have graylevel values 1 and 0 respectively. Both

bands have Gaussian noise with standard deviation 0.5 added. Figure 1 shows the two bands without noise in the first column, the two bands with noise in the second column, the CEM results for end-members $[1\ 0]^T$ (horizontal bar) and $[0\ 1]^T$ (vertical bar) stretched linearly from minimum to maximum in the third column, and the CEM results stretched linearly from 0 to 1 in the fourth column.

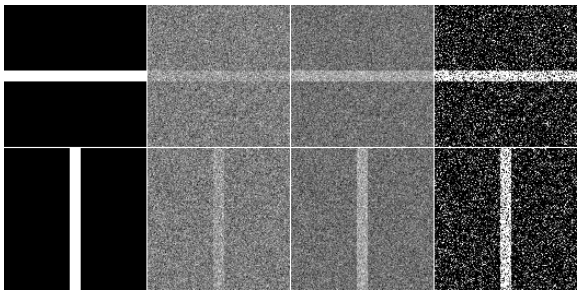

Figure 1: Two bands simulated (without noise in column one, with noise in column two) and the CEM result (columns three and four)

5.2 AVIRIS data over the Mojave Desert, California, USA

The data used here is the 30 bands subset of AVIRIS, [20], data over a small part of the Mojave Desert, California, USA, that come with the LinkWinds software, [7]. These bands cover the spectral range 0.52–2.33 μm. The images have 180 rows and 360 columns.

To establish which regions in the image contain extreme values and therefor are potential end-members we look for the minimum and maximum values in the MAFs. Figure 2 shows every other of the 30 bands and the first 14 MAFs (row-wise). Since we don't want our partial unmixing results to be based on noise spectra we use training areas grown from the pixels with extreme values as seeds to calculate average spectra instead of using the spectra from the pixels themselves directly.

This is a "true remote sensing situation," we don't know what is on the ground. Our aim here is to illustrate the CEM method and not to classify or identify material on the ground. We arbitrarily choose six potential end-members corresponding to the extreme values of MAFs 1-3.

Figure 3 shows the six training areas grown from these extremes by `seed`. Figure 4 shows the resulting abundance images as estimated from the first 9 MAFs by CEM.

6 CONCLUSIONS

CEM and an eigenvalue formulation alternative enable us to perform partial unmixing when we know the desired end-member spectra only and not the full set of end-member spectra. This is an advantage over full unmixing and OSP. When applying the CEM method or the eigenvalue formulation alternative to MAFs or MNFs, matrix inversion is not needed and also the noise isolated in the MAF/MNFs not included in the analysis does not influence the matched filtering performed.

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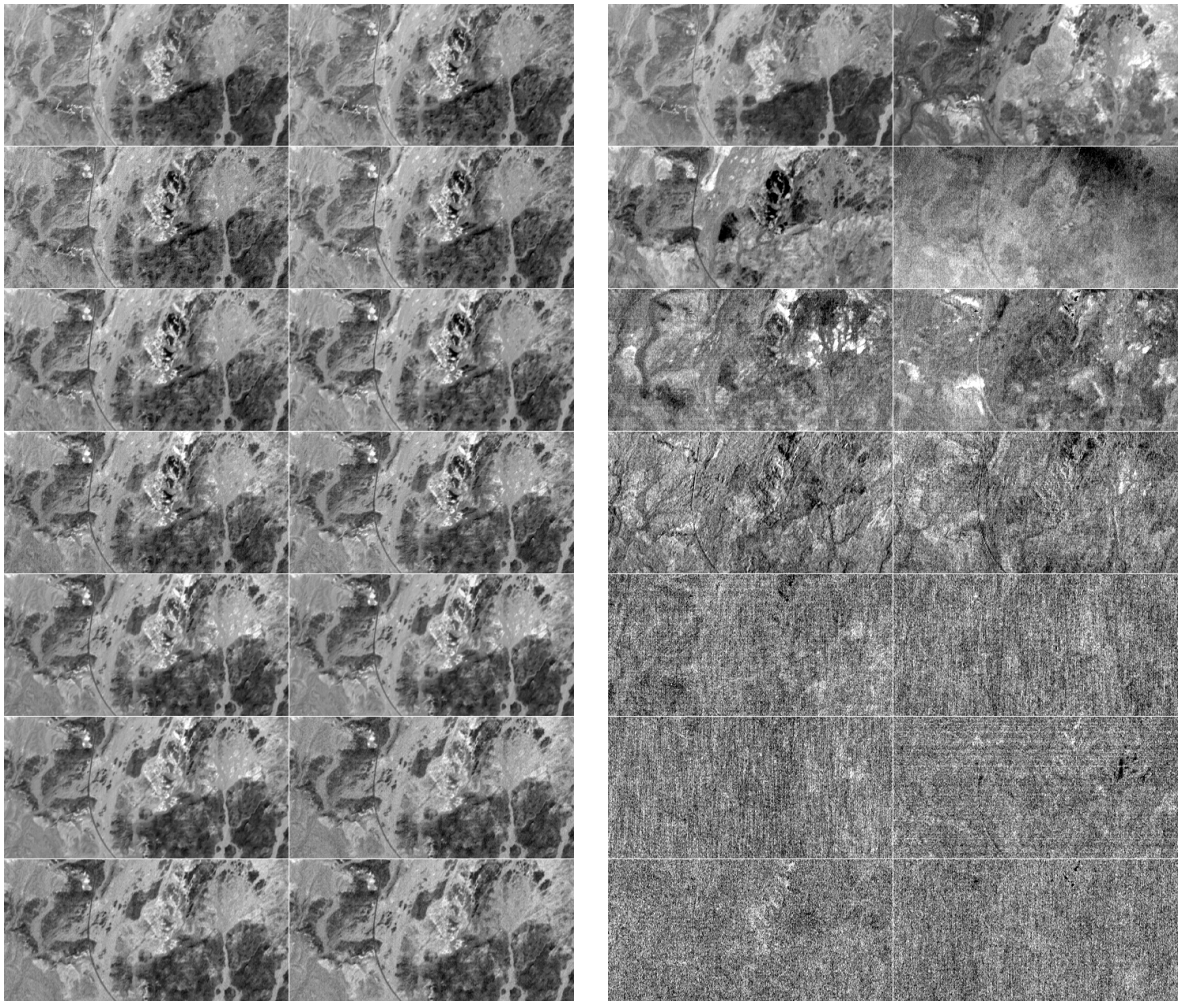

Figure 2: Every other of the 30 bands subset of AVIRIS data over the Mojave Dessert, California, USA (left); the first 14 MAFs of the AVIRIS data (right)

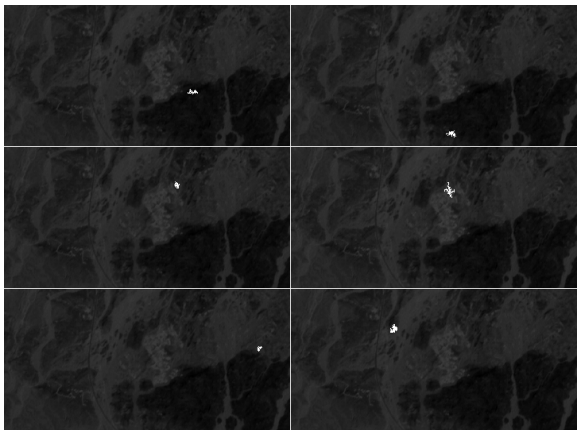

Figure 3: Seed grown training areas under which average spectra are calculated shown in white on top of MAF1 (see Figure 2)

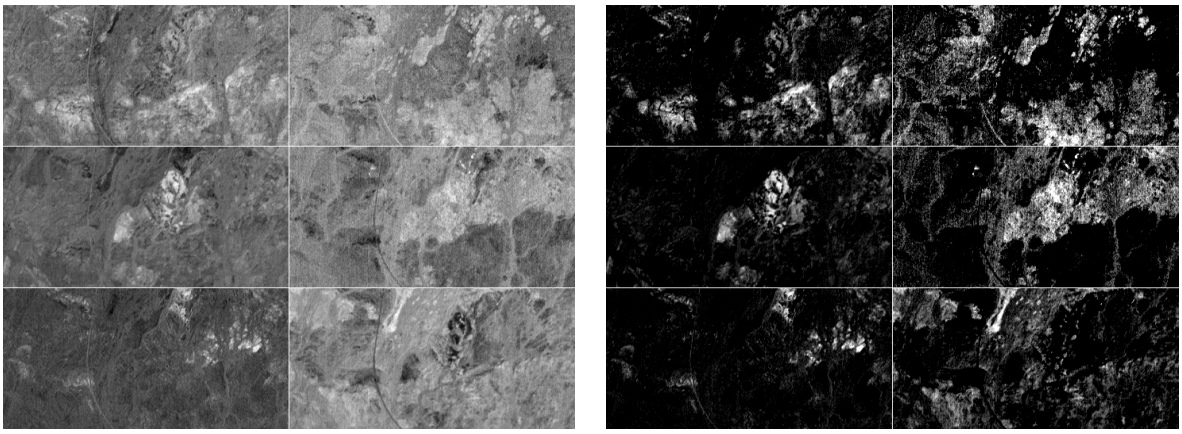

Figure 4: CEM abundance estimates stretched linearly from minimum to maximum (left); stretched linearly from 0 to 1 (right)

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