This item is the archived peer-reviewed author-version of:

Robust supervised method for nonlinear spectral unmixing accounting for endmember variability

Reference:

Koirala Bikram, Zahiri Zohreh, Lamberti Alfredo, Scheunders Paul.- Robust supervised method for nonlinear spectral unmixing accounting for endmember variability
IEEE transactions on geoscience and remote sensing / Institute of Electrical and Electronics Engineers [New York, N.Y.] - ISSN 0196-2892 - (2020), p. 1-15
Full text (Publisher's DOI): <https://doi.org/10.1109/TGRS.2020.3031012>
To cite this reference: <https://hdl.handle.net/10067/1740280151162165141>

Robust supervised method for nonlinear spectral unmixing, accounting for endmember variability.

Bikram Koirala, *Student Member IEEE*, Zohreh Zahiri, *Member IEEE*, Alfredo Lamberti, Paul Scheunders, *Senior Member IEEE*

Abstract—Due to the complex interaction of light with mixed materials, reflectance spectra are highly nonlinear mixtures of the reflectances of the pure materials that are contained within a mixed pixel, making it hard to estimate the fractional abundances of the materials. Changing illumination conditions and cross-sensor situations cause endmember variability, further complicating the unmixing. In this work, we propose a supervised approach to unmix mineral powder mixtures, containing endmember variability. The method combines a supervised regression method to learn the nonlinearity with a geodesic distance-based approach, that is invariant to endmember variability. Experiments are conducted on simulated and real mineral mixtures. In particular, we developed datasets of homogeneously mixed mineral powder mixtures, acquired by 2 different sensors, an Agrispec spectrometer and a snapsan shortwave infrared hyperspectral camera, under strictly controlled experimental settings. The proposed approach is compared to other supervised approaches and nonlinear mixture models.

Index Terms—Hyperspectral, mixing models, mineral powder mixtures, machine learning regression

I. INTRODUCTION

The goal of spectral unmixing is to estimate the fractional abundances of the different pure materials (endmembers) that are contained within a hyperspectral pixel. Generally, spectral unmixing is performed by defining a mathematical model that describes the spectral reflectance as a function of the endmembers and their fractional abundances. The inversion of that model then gives an estimation of the pixels composition.

Among all mathematical models, the linear mixing model (LMM)[1] is the most popular one. This model assumes that each incoming ray of light interacts only once with a specific pure material in the pixel before reaching the sensor. When taking into account the physical non-negativity and sum-to-one constraints of the fractional abundances, the fully constrained least squares unmixing (FCLS)[2], [3] procedure can be applied to minimize the error between the true and the reconstructed spectrum.

The LMM produces large errors when the hyperspectral dataset is obtained from complex geometrical structures or intimate mixtures. In these scenarios, the incident ray of light interacts with several pure materials within a hyperspectral pixel before reaching the sensor. There exist several nonlinear mixing models that model multiple interactions [4]. The bilinear models ([4], [5]) extend the LMM by adding

bilinear terms, allowing the incident ray to interact with two pure materials before reaching the sensor. Other models extend these towards multiple interactions, e.g., the multilinear mixing model (MLM)[6] and the p-linear ($p > 2$) mixing model (pLMM)[7], [8], [9].

The most advanced nonlinear mixing models are physics-based radiative transfer models. These models are often employed for modeling intimate mixtures of materials. They represent the medium as a half-space filled with particles with known densities and distributions of physical attributes. The Hapke model is a simplified version of a radiative transfer model and was developed to explain the interaction of the light with intimately mixed materials [10], [11].

Instead of depending on a particular mixing model for spectral unmixing, some attempts have been made to learn the nonlinearity of the dataset using a data-driven approach. Algorithms were developed that performed the spectral unmixing in a reproducing kernel Hilbert space [12], [13]. Radial basis function kernels were used to kernelize FCLS (KFCLS), but no improvement in the unmixing of intimate mixtures was observed [14], [15].

Supervised spectral unmixing methods were developed that require ground truth fractional abundances of a number of training spectra [16], [17], [18], [19], [20]. These methods apply the ground truth as training data to learn the nonlinear relationship between the measured spectra and the fractional abundances. One disadvantage is that a direct mapping to the abundances is unconstrained and does not guarantee that the obtained results correspond to the actual fractions. To solve this issue, in [21], [22], a mapping of the nonlinear spectra to the linear model was learned with machine learning regression algorithms, after which FCLS was applied to estimate the fractional abundances.

A major disadvantage of the supervised methods is their generalizability. When the training and test samples lie on different data manifolds, the performance of this methodology decreases. This occurs in any situation containing spectral variability. There exist several algorithms that consider endmember variability: algorithms based on endmember bundles, computational models, and parametric physics-based models ([23], [24]). All these methods however were only applied on linearly mixed datasets. The situation is much more complex when the endmembers are mixed nonlinearly.

There exist different types of spectral variability. External spectral variability is caused by variable acquisition conditions, i.e. variable illumination conditions, distance and orientation from the sensor [25]. These effects cause a scaling of the spectral reflectance. Although the nonlinearity of the data

Bikram Koirala, Zohreh Zahiri and Paul Scheunders are with the Imec-VisionLab, Department of Physics, University of Antwerp, Belgium e-mail: {bikram.koirala, zohreh.zahiri, paul.scheunders}@uantwerpen.be

Alfredo Lamberti is with the ENGIE Laborelec, Linkebeek, Belgium e-mail: alfredo.lamberti@engie.com

manifold does not change with scaling, nonlinear models are not invariant to scaling, since the spectral reflectance is a nonlinear function of the endmembers and fractional abundances.

Another type of external variability may occur between different datasets, e.g. obtained from different sensors, or when different white calibration panels are used. These effects cause a wavelength dependent scaling of the spectra, for which nonlinear models are not invariant. It is assumed that these effects are small compared to the global scaling effects.

Intrinsic spectral variability occurs when the material composition changes from one mixture to another, e.g. caused by variable grain size distributions. This is expected to change the nonlinear behavior of the manifold. In this work, intrinsic variability is assumed to be absent and is not considered.

The literature reports only limited research devoted to the treatment of spectral variability in nonlinear unmixing. [26] proposes a band-wise scaling of the LMM to model either spectral variability in the linear case or nonlinear mixing. In [27], [28], bilinear models were extended with a scaling term to tackle external spectral variability. In [29], endmembers were modeled by a normal distribution to reduce the influence of endmember variability in bilinear models. In [30], a multi-type mixing model was proposed to handle nonlinear unmixing and spectral variability for the purpose of HSI reconstruction.

In general, inversion of a model that treats spectral variability and nonlinearity simultaneously is highly non-convex. Most of the proposed models have large amounts of hyperparameters, making an abundance estimation hard. Moreover, relying on one particular model makes a method inflexible in e.g. cross-sensor situations.

In this work, we will develop a supervised model-independent approach to handle spectral variability for nonlinear unmixing. The method uses a geodesic distance-based unmixing approach [31] to tackle the spectral variability. This approach can be shown to be invariant to global scaling and thus to external spectral variability. It can predict fractional abundances (latent variables) of the nonlinear dataset accurately when the curvature of the manifold is constant. This is unfortunately not the case in nonlinearly mixed data, where the geodesic distance will be nonlinearly related to the fractional abundance. For this, the approach is combined with a supervised nonlinear regression method, to learn the nonlinear relationship between the abundances estimated by the geodesic approach and the actual ones.

The major disadvantage of supervised methods is that they require ground truth data. Very limited research has been devoted to producing ground truth data for spectral unmixing tasks [32]. Most of the spectral unmixing tasks are focused on estimating fractional abundances from airborne or satellite hyperspectral images. To produce unmixing ground truth data for these images is difficult. This restricts the validation of the developed algorithms on real datasets to visual interpretations.

Recent developments in compact, low-cost hyperspectral sensors, allow to produce hyperspectral datasets in laboratory settings. To validate our strategy, we produced a hyperspectral dataset of mineral powder mixtures. To include spectral variability, we acquired the spectra by two different sensors, an

Agrispec spectrometer and a snapscan shortwave infrared hyperspectral camera. Both the images/spectra of pure minerals and their mixtures are available. To the best of our knowledge, this dataset is the first publicly available dataset captured by two independent sensors. Experiments on the Relab mineral mixture dataset will also be performed.

The remaining of the paper is organized as follows: In Section II, the proposed methodology is elaborated. In section III, we describe the datasets on which our methodology is validated. In Section IV, we describe the experiments and the results, followed by a discussion in Section V. Section VI concludes this work.

II. SUPERVISED GEODESIC DISTANCE-BASED UNMIXING

A. Hyperspectral mixing models

Before describing the proposed approach, in this section, we first fix some notations and describe a few mixing models. Let $\mathbf{E}(\{\mathbf{e}_j\}_{j=1}^p \in \mathbf{R}_+^d)$ be a set of p endmembers (i.e., pure spectra) composed of d spectral bands. Suppose that N samples contain mixtures of these endmembers, with fractional abundances denoted by the matrix $\mathbf{A}(\{\mathbf{a}_i\}_{i=1}^N \in \mathbf{R}_+^p)$. It is generally assumed that the spectral reflectances of these N samples, $\mathbf{Y}(\{\mathbf{y}_i\}_{i=1}^N \in \mathbf{R}_+^d)$ are generated by a nonlinear function F of the endmembers and fractional abundances:

$$\mathbf{y}_i = F(\mathbf{E}, \mathbf{a}_i) + \boldsymbol{\eta}_i, \quad (1)$$

where $\boldsymbol{\eta}_i$ represents Gaussian noise. Each mixing model corresponds to a particular choice of F .

1) *Linear mixing model (LMM)*: The linear mixing model assumes that $\mathbf{Y}$ is written as:

$$\mathbf{Y} = \mathbf{E}\mathbf{A} + \mathbf{N}, \quad (2)$$

where $\mathbf{N}$ represents the matrix containing gaussian noise. When assuming that the fractional abundances are non-negative and sum-to-one, the fully constrained least squares unmixing algorithm (FCLSU) can be applied to estimate the fractional abundances. FCLSU minimizes $\|\mathbf{y}_i - \mathbf{E}\mathbf{a}_i\|^2$ s.t. $\sum_j a_{ji} = 1, \forall j : a_{ji} \geq 0$.

2) *Fan model*: Bilinear models have been designed to allow for secondary reflections. In [5], the Fan model is derived by the first-order Taylor series expansion of a general nonlinear mixing function:

$$\begin{aligned} \mathbf{y}_i &= F(\mathbf{E}, \mathbf{a}_i) + \boldsymbol{\eta}_i \\ &= \mathbf{E}\mathbf{a}_i + \sum_{j=1}^{p-1} \sum_{k=j+1}^p a_{ji}a_{ki}\mathbf{e}_j \odot \mathbf{e}_k + \boldsymbol{\eta}_i \end{aligned} \quad (3)$$

where $\odot$ is the elementwise multiplication of two vectors.

3) *Hapke model*: The Hapke model [10], [11] describes the optical characteristics of intimately mixed materials. This model assumes that the particles have a size, much larger than the wavelength of the light, are of similar shape, and are randomly oriented. In general, this model needs information regarding the physical state of the surface (particle size, surface roughness, etc.), the real and imaginary parts of the optical indexes, and the viewing geometry. In [33], it was simplified for remote sensing applications. This simplified version of the

Hapke model relates the bidirectional reflectance $\mathbf{Y}$ with the single scattering albedos (SSA) $\mathbf{W}(\{\mathbf{w}_i\}_{i=1}^N \in \mathbf{R}_+^d)$ by the following equation:

$$\begin{aligned} \mathbf{Y} &= F(\mathbf{E}, \mathbf{A}) \\ &= \frac{\mathbf{W}}{(1 + 2\mu\sqrt{1 - \mathbf{W}})(1 + 2\mu_0\sqrt{1 - \mathbf{W}})}, \end{aligned} \quad (4)$$

where $\mu = \cos(\theta_e)$ and $\mu_0 = \cos(\theta_i)$ are the cosines of the angles with the normal of the outgoing and incoming radiation respectively. While the reflectance of intimately mixed materials does not follow the linear mixing model, the SSA do follow it:

$$\mathbf{w}_i = \mathbf{W}^E \mathbf{a}_i, \quad (5)$$

where $\mathbf{W}^E(\{\mathbf{w}_j^E\}_{j=1}^p \in \mathbf{R}_+^d)$ denotes the SSA of the endmembers.

B. Step 1: Geodesic distance-based unmixing

Following a geometric description of the LMM, the data manifold is a simplex, spanned by the endmembers which form a linear basis for the mixed pixel spectra. Many unmixing algorithms exploit this geometric notion. With this description, the spectral unmixing can be described in a distance-based manner, in which the fractional abundances a_j of a data point $\mathbf{y}$ can be written as:

$$a_j = \frac{V(\mathbf{e}_1, \dots, \mathbf{y}, \mathbf{e}_{j+1}, \dots, \mathbf{e}_p)}{V(\mathbf{e}_1, \dots, \mathbf{e}_p)} \quad (6)$$

i.e., the volume of the simplex obtained by replacing the j^{th} vertex by $\mathbf{y}$, divided by the total volume of the largest simplex. The volume of a simplex is calculated as:

$$\begin{aligned} V(\mathbf{e}_1, \dots, \mathbf{e}_p) &= \sqrt{\frac{(-1)^p \cdot \text{cmd}(\mathbf{E})}{2^{p-1}(p-1)!}}, \quad \text{with} \\ \text{cmd}(\mathbf{E}) &= \det \begin{pmatrix} 0 & 1 & 1 & 1 & \dots & 1 \\ 1 & 0 & d_{1,2}^2 & d_{1,3}^2 & \dots & d_{1,p}^2 \\ 1 & d_{2,1}^2 & 0 & d_{2,3}^2 & \dots & d_{2,p}^2 \\ 1 & d_{3,1}^2 & d_{3,2}^2 & 0 & \dots & d_{3,p}^2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & d_{p,1}^2 & d_{p,2}^2 & d_{p,3}^2 & \dots & 0 \end{pmatrix} \end{aligned} \quad (7)$$

where cmd denotes the Cayley–Menger determinant and $d_{m,k}^2$ is the (Euclidean) distance between endmembers $\mathbf{e}_m$ and $\mathbf{e}_k$.

In, [31], this geometric concept was extended to nonlinear manifolds, where the Euclidean distance can be replaced by the geodesic distance (see Fig. 1). A well-known data-driven approach for approximating geodesic distances on a manifold is constructing a nearest neighbor graph on the data. The geodesic distance between any two points is then defined as the shortest-path distance along the graph (i.e. using locally the Euclidean distance between neighboring points on the graph) between these two points. The Dijkstra algorithm [34] can be used to calculate the shortest-path distances. These distances will approximate the true geodesic distances as measured along the surface of the data manifold.

Let us focus on binary mixtures from now on. The manifold sampled by a number of binary mixtures of two materials is a curve in spectral space between the two endmembers. The

Fig. 1: A data point $\mathbf{y}$ lies inside the nonlinear simplex spanned by $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$. The fractional abundance a_j is equal to the volume ratio V_i/V , with $V = \sum_j V_j$.

curve can then be approximated by a piece-wise linear curve and the geodesic distance is then simply approximated by the sum of the Euclidean distances between neighboring samples on the 1-NN graph. For this, it is important to correctly order these samples. This can be done by generating a distance matrix, containing the distances from each point to any other point, start from an endmember and iteratively look for the next closest point. The more mixture samples are available, the better the approximation. In some practical situations, only mixture (and the 2 endmembers) may be available, so that the approximation leads to errors. However, since the degree of the manifold curves is expected to be low, the errors are limited to a few percent.

For the geodesic distance leading to the correct fractional abundances, the data manifold should have a small non-zero constant curvature. In that case, the arc length between the endmembers and the mixture along the manifold is proportional to the fractional abundance. This is the case, e.g. for a circle and a helix, but not so for a parabola. It is very unlikely that a real data manifold will satisfy this condition. The fractional abundances estimated by geodesic unmixing for datasets generated by the bilinear models or the Hapke model have a nonlinear relationship with the true fractional abundances. In Appendix A, this is illustrated for the Fan model.

To further demonstrate this, we simulated a data manifold of binary mixtures of Bronzite and Calcite, for which the endmember spectra are obtained by the USGS library (Fig. 2 (a)). The ground truth fractional abundances were generated uniformly from the unit simplex and mixtures were simulated according to the Hapke model. In Fig. 2 (c), the true fractional abundance is plotted against the estimated fractional abundance by geodesic unmixing.

Despite the fact that the geodesic distance-based unmixing produces large errors in estimating fractional abundances of nonlinear hyperspectral datasets, the main advantage of this approach is that it is invariant to global scaling of the manifold, and thus invariant to external variability, caused by variable acquisition conditions. To illustrate this, we scale the Bronzite-

Fig. 2: (a) Endmember spectra of Bronzite and Calcite; (b) True data manifold and scaled versions. The dashed lines represent the data manifold, generated by the Hapke model; (c) The true fractional abundance of Calcite against the one estimated by geodesic unmixing. (d) The true fractional abundance of Calcite against the one estimated by the Hapke model.

Calcite manifold (Fig. 2 (b)) and again plot the estimated against the true abundances (Fig. 2 (c)). As can be observed, the estimated geodesic abundances remain invariant.

Nonlinear models however are not invariant to such scaling. To demonstrate this, Fig. 2 (b) shows that the data manifolds, generated by the Hapke model from the scaled endmembers do not follow the scaled manifold. Fig. 2 (d) plots the obtained abundances by Hapke against the true ones. As can be observed, the performance of the Hapke model for estimating the fractional abundances drops significantly on the scaled manifolds.

This demonstrates that the geodesic distance approach produces incorrect abundances but is able to reveal the underlying nonlinearities, which remain the same after scaling the manifold. Let us denote the estimated geodesic fractional abundances by $\hat{\mathbf{A}}(\{\hat{\mathbf{a}}_i\}_{i=1}^N \in \mathbf{R}_+^p)$.

C. Step 2: Machine learning regression

In order to derive the correct abundances from the estimated ones by geodesic unmixing, we will resort to a supervised approach. To this aim, we assume that a set of n training samples with known fractional abundances: $\mathcal{D} = \{(\mathbf{y}_1, \mathbf{a}_1), \dots, (\mathbf{y}_n, \mathbf{a}_n)\}$ is available. The proposed procedure is the following:

- To account for the constraints, linearly mixed training spectra $\mathbf{X}_{\mathcal{D}} = \{\mathbf{x}_i\}_{i=1}^n$ are generated from the ground truth abundances and the endmembers:

$$\mathbf{x}_i = \mathbf{E}\mathbf{a}_i, \forall i \in \{1, \dots, n\}. \quad (8)$$

- Then, a map is learned from the geodesic abundances of the training set $\hat{\mathbf{A}}_{\mathcal{D}} = \{\hat{\mathbf{a}}_i\}_{i=1}^n$, obtained from step

1 in the procedure, to the generated linearly mixed spectra $\mathbf{X}_{\mathcal{D}}$. Any nonlinear regression method can be applied to train such a model. In this work, we choose Gaussian Processes regression [35] as a machine learning algorithm.

- After learning the map, the obtained regression model is applied to map the geodesic abundances of the test data $\hat{\mathbf{A}}_t = \{\hat{\mathbf{a}}_t\}_{t=n+1}^N$ to linearly mixed spectra $\mathbf{X}_t = \{\mathbf{x}_t\}_{t=n+1}^N$.
- Once the mapping is learned and the test spectra are mapped onto the linear spectra, the final step is to obtain the fractional abundances from the mapped linear spectra, by inverting the LMM model.

Step 2 of the procedure is similar to a mapping of the observed spectra directly to the fractional abundances [16], [17], [18], [19], [20], or to the linear model [22]. The main disadvantage of these approaches from the literature is that the performance decreases when the training and test samples are from the two different data manifolds. This happens when the training and test samples are captured by two independent sensors. This also happens when the illumination conditions on the training and the test samples are not entirely similar. In general, the variability of the endmembers produces different data manifolds. When the underlying nonlinearity is the same for the two different data manifolds, geodesic unmixing should produce identical fractional abundances for both of them. For this reason, we introduce the geodesic unmixing of step 1 before learning the mapping to the linear model. Fig. 3 illustrates the proposed methodology. We will refer to this approach as geodesic supervised unmixing(GSU).

Fig. 3: Flowchart of the proposed method.

III. DATA

A. Dataset 1: Self-crafted mineral dataset

For the validation of our proposed method, we created a data set, containing in total 49 binary mixtures of mineral powders. The five chosen minerals are different oxides, typically found in soil, and applied in cementitious materials: Aluminum oxide (Al_2O_3), Calcium oxide (CaO), Iron oxide (Fe_2O_3), Silicon dioxide (SiO_2) and Titanium dioxide (TiO_2). The degree of purity of all minerals was above 98%. All mineral powders have a white color (except for Iron oxide which is red) and have different densities and grain sizes (see Table I).

TABLE I: Density and grain size (D50) of the minerals used in the self-crafted mineral dataset.

Mineral	Density (g/cm ³)	Grain size (μm)
Al ₂ O ₃	3.98	3.5
CaO	3.34	2.7
Fe ₂ O ₃	5.26	0.8
SiO ₂	2.64	23
TiO ₂	3.89	0.5

In total, 7 binary mixture combinations of minerals were prepared: Al₂O₃-SiO₂ (Al-Si), CaO-SiO₂ (Ca-Si), CaO-TiO₂ (Ca-Ti), Fe₂O₃-Al₂O₃ (Fe-Al), Fe₂O₃-CaO (Fe-Ca), Fe₂O₃-SiO₂ (Fe-Si) and SiO₂-TiO₂ (Si-Ti). For each mineral combination, 7 different mixtures were prepared. We fixed the weight of each mixture to be in total 10 g (the scale had an accuracy of 0.001 g), and increased the weight of the first endmember in the mixture by a fixed step of 1.25 g, from 1.25 g to 8.75 g. We then converted the weight to areal fraction, based on the known density and grain size of each pure material. For the case of tightly packed spherical particles, the areal fraction of each material can be written as follows:

$$a_j = \frac{\frac{M_j}{\rho_j D_j}}{\sum_{j=1}^p \frac{M_j}{\rho_j D_j}}, \quad (9)$$

where M_j is the mass fraction of component j , ρ_j its density, and D_j its average diameter.

Since the grain sizes and densities vary between the minerals, and the grain sizes are of the same order as the SWIR wavelength range, it can be expected that the Hapke model will not provide accurate areal fractional abundance estimates.

1) *Sample preparation*: Before mixing the minerals, they were grinded to avoid clusters of grains causing inhomogeneities. The minerals were then put inside a glass container and mixed by rotating the container for approximately 5 minutes to guarantee a homogeneous mixture. Each mixture was then put inside a round black sample holder with an interior diameter of 20 mm, a height of 5.5 mm, and an edge thickness of approximately 3 mm. The sample holder was completely filled and compacted and smoothened using a tamp compactor. Each sample was scanned 3 times, each time emptying and refilling the sample holders.

The samples were scanned with two different instruments: a snapscan hyperspectral SWIR camera (manufactured by Imec) and an AgriSpec spectrometer (manufactured by ASD (Analytical Spectral Devices)).

2) *Scanning setup of hyperspectral camera*: The spectral range of the camera is 1100-1670 nm with a spectral resolution of approximately 5 nm, resulting in a total of 113 spectral bands (the first 10 bands were very noisy and were discarded). In contrast to pushbroom systems, in which either the camera or the sample should move, in the snapscan camera the sensor moves inside the camera, allowing to acquire a still full image frame.

The samples were located in a region of 2cm² in the center of the camera's FOV to guarantee the lowest spectral variability. Four halogen lamps (20W GU5.3 cool-fit) with diffusers were used for a hemispherical-directional illumina-

tion to simulate uniform real-world solar illumination. The distances of the sample to the halogens and the camera were approximately 30 cm and 40 cm, respectively. During scanning, the lights inside the room were turned off. Each image scan took approximately 45 seconds.

The original frame size of the raw images was 150 × 150 pixels. To provide data with uniform illumination and remove unrelated objects (edge of the sample holders) the images were clipped to 30 × 30 pixels. Since all mixtures were homogeneous, no spatial variation between the spectra was observed, and the spectra of all pixels were averaged over the entire clipped image.

3) *Scanning setup of spectrometer*: The data from the spectrometer have 1500 spectral bands, ranging from 1000 nm to 2500 nm with a step size of 1 nm. The wavelength range was clipped to the range of the hyperspectral camera, leaving 570 bands, from which the first 44 were noisy and discarded. The sensor is placed in a muglight for maximum illumination and sample stability, required for a good signal-to-noise ratio and to minimize measurement errors associated with stray light and specular reflected components. The muglight was mounted on top a box with a hole in the middle (slightly larger than the size of the sample holder), in order to place and remove the sample holders easily under the muglight. Every sample was individually held under the muglight for scanning from a fixed distance. The size of the scanning area in the spectrometer was 25 mm, thus positioning the edge of the sample holder in the field of view of the spectrometer. Since the spectrum of the sample holder was flat and close to zero in the entire spectral range of the spectrometer, this resulted in a slightly lower spectral reflectance. A slight horizontal degree of freedom resulted in a scaling effect on the acquired spectra. Three spectra were collected from each sample and by repeating the measurements 3 times (after emptying and refilling the sample holders), this resulted in 9 spectra for each sample.

Figure 4 shows the spectra of the pure materials acquired by both the spectrometer and the camera. A substantial difference between the acquired spectra can be observed, due to external variability, including variation in illumination and distance of the samples from the sensor, causing global scaling effects, and sensor-related differences, such as the use of different white-calibration, causing wavelength dependent scaling. Although we could correct for the latter, by applying the same calibration panel in both cases, we deliberately did not, to provoke cross-sensor differences.

The dataset and the trained models generated by the proposed method on this dataset are publicly available at "<https://github.com/VisionlabUA/Mineral-dataset>".

B. Dataset 2: RELAB dataset

This data set contains spectra of crafted mineral mixtures from the NASA Reflectance Experiment Laboratory (RELAB) at Brown University, publicly available at www.planetary.brown.edu/relab/ [36]. From the data set, binary mixtures from five minerals: Anorthite (An), Bronzite (Br), Olivine (Ol), Quarts (Qz) and Alunite (Al) were chosen. For the binary mixtures of

Fig. 4: Spectra of the pure minerals acquired by the spectrometer (black line) and hyperspectral camera (blue line).

An-Br, Br-Ol, Ol-An and Qz-Al, each time 3 mixtures were available with a 25%, 50% and 75% ratio by mass. These minerals have equivalent grain sizes (of the order of $100 \mu\text{m}$) and densities (around 3 g/cm^3), making the volumetric and areal fractional abundances very close to these mass ratio's. The actual areal fractions are shown in the results section in Table VI. The main reason for selecting these four binary mixtures is that the fractional abundances are accurately estimated by the Hapke model.

In order to validate the supervised approaches, a training data set is required. Moreover, we want to assess the ability of the proposed method to account for endmember variability. Therefore, we obtained endmembers for the five minerals from the USGS spectral library of minerals (<https://speclab.cr.usgs.gov/spectral-lib.html>). Endmembers from both USGS and Relab are shown in Fig. 5. It can be observed that the endmember spectra are quite different, since these endmembers were independently acquired by different sensors, and the used samples may exhibit some intrinsic variability as well. For the four binary mixtures, uniformly distributed ground truth fractional abundances were generated (100 in total). Then, nonlinear spectra were artificially generated by applying the Hapke model on the USGS endmembers.

Finally, the mineral mixtures Calcite-Chlorite (Cal-Chl) were obtained both from the USGS library and the Relab dataset. The Relab dataset contains three mixtures of Calcite and Chlorite (25 %, 50% and 75% by mass respectively) while the USGS library dataset contains two mixtures (33% and 66% by mass).

Fig. 5: Endmembers obtained from the USGS library (dashed) and the Relab dataset (full line).

IV. EXPERIMENTS AND RESULTS

The proposed method GSU was validated and compared to 3 unsupervised models, unsupervised geodesic unmixing and 2 other supervised approaches:

- LMM: the linear unmixing model
- Fan: a bilinear mixture model
- Hapke: the Hapke model
- GU: unsupervised geodesic unmixing. This is the first step of the proposed approach only.
- SM: a softmax feedforward neural network to estimate the fractional abundances. This method is similar to the second step of the proposed procedure. It is a supervised approach that uses a training set to learn a direct mapping of the observed spectra to the actual fractional abundances. In this network, the input layer contains d nodes, representing the spectral bands of the actual spectra. There is one hidden layer consisting of $h = 5$ nodes and the output layer consisting of p nodes, containing the true fractional abundances. The hyperbolic tangent function ($\tanh(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}$) is used as an activation function for the hidden layer and the softmax activation ($f(a_j) = \frac{\exp(a_j)}{\sum_{j=1}^p \exp(a_j)}$) for the output layer. This activation function guarantees the positivity and sum-to-one constraints on the abundances.
- GP_LMM: This supervised method learns a mapping from the observed spectra to the linear model [22]. As the mapping procedure, Gaussian Processes is applied. In contrast to the proposed method, GP_LMM does not account for spectral variability and will not properly work in cross-sensor situations. Some endmember variability can however be taken into account by applying the learned mapping to map the endmember spectra of the test dataset to the endmember spectra of the training dataset, a procedure that cannot be performed with the direct mapping method SM.

A phenomenon that was observed in most of the applied data was a random scaling of the spectra, due to variations in

the acquisition conditions. For example, since the height of the sample holder was not easily controllable in the spectrometer, the self-crafted mineral mixtures were scaled with respect to each other in a random manner. This phenomenon does not cause problems on the mixing models, but leads to ordering problems in the geodesic unmixing approach and to mapping errors in the supervised approaches. A normalization of all spectra by their length (i.e. a projection onto the unit circle), prior to the application of an unmixing procedure would solve this issue. For this reason, we will normalise the spectra in all experiments prior to applying the methods GU, SM, GP_LMM and the proposed method GSU.

It is important to notice that this projection is nonlinear, and thus changes the nonlinearity of the manifolds. This will introduce errors in the geodesic unmixing approach. In the supervised approaches however, it does not introduce extra errors, since the nonlinearity is changed both in the training and the test manifolds in a similar way.

All quantitative comparisons are provided by the abundance root mean squared error (RMSE), i.e. the error between the estimated fractional abundances ($\hat{\mathbf{A}}$) and the ground truth fractional abundances ($\mathbf{A}$):

$$\text{Abundance RMSE} = \sqrt{\frac{1}{pn} \sum_{k=1}^p \sum_{i=1}^n (\hat{\mathbf{A}}_{ki} - \mathbf{A}_{ki})^2} \times 100 \quad (10)$$

where p and n denote the number of endmembers and the number of mixed spectra respectively.

A. Experiments on self-crafted mineral dataset

1) *Experiment 1: Simulated manifolds:* In the first experiment, we generated simulated manifolds using the measured mineral endmembers from the camera and the spectrometer. From the mineral endmembers obtained from the AgriSpec spectrometer, ground truth fractional abundances were generated uniformly from the unit simplex. Then, nonlinear spectra were artificially generated by applying the Fan and the Hapke model, respectively. In this way, ten binary mixtures: (Al-Ca), (Al-Fe), (Al-Si), (Al-Ti), (Ca-Fe), (Ca-Si), (Ca-Ti), (Fe-Si), (Fe-Ti) and (Si-Ti) were produced for each of both mixing models. Similarly, simulated manifolds were produced from the mineral endmembers obtained from the camera. Some of the data manifolds from both the spectrometer and camera are shown in Fig. 6. As can be observed from the figure, the manifolds simulated by the Fan and Hapke models are quite different, and applying one model on the manifold generated by the other model will not work. Also, the application of the linear model is expected to lead to large errors, in particular for the Fan manifolds. In the Al-Fe mixture, half of the manifold will be projected onto the second endmember. Another observation is that the manifolds of the camera and the spectrometer are obviously different, since also the endmembers are different (see Fig. 4).

In Table II, the abundance RMSEs of the simulated camera data are shown. Obviously, the Fan model results are not shown on the simulated Fan data and the Hapke model results are not shown on the simulated Hapke data. The supervised

Fig. 6: Manifolds of the simulated spectrometer dataset (black dots) and the simulated hyperspectral camera dataset (blue dots), generated by the Fan model and the Hapke model.

algorithms were trained on the simulated spectrometer dataset. The geodesic distance was calculated by using all samples on the manifold. The outcomes of the experiments can be summarized as follows:

- As expected, the performance of the unsupervised models is poor, since the manifolds of the simulated Hapke and Fan data are completely different. As an exception, the linear model performs quite well on the Hapke dataset, because the manifolds are close to linear.
- The geodesic distance estimation of the abundances leads to errors of about 10% on the Fan data. On the Hapke data, it performs as well as the linear model, since the manifolds are close to linear. The errors are caused by the fact that the manifolds have a non-constant curvature.
- From the supervised approaches, the performance of SM is poor for any of the mixtures. This demonstrates that a direct mapping from the observed spectra to abundances will not work in a cross-sensor situation.
- The results of GP_LMM are much better, since this method also maps the endmembers. Results however are clearly better for the Hapke data and vary a lot between mixtures.
- Overall, the proposed approach GSU produces less than 2% abundance RMSE for most of the simulated binary mixtures. The proposed method is found to be very robust to endmember variability in the cross-sensor situation.

2) *Experiment 2: Single sensor unmixing:* In the second experiment, we investigated the performance of the supervised methods when trained and tested on the data from the same sensor. For this, the real mixtures were applied. 4 of the 7 mixtures (with 1.25, 3.75, 6.25 and 8.75 g of the first mineral respectively) were applied for training and the other 3 (2.5, 5.0 and 7.5 g) for testing. Results are shown in Table III for the camera data and Table IV for the spectrometer data. For comparison, the results of the unsupervised approaches are

TABLE II: Abundance RMSE in %. Algorithms were trained on the simulated spectrometer data and tested on the simulated hyperspectral camera data.

Binary Mixture	Fan LMM	Fan Hapke	Fan GU	Fan SM	Fan GP_LMM	Fan GSU	Hapke LMM	Hapke Fan	Hapke GU	Hapke SM	Hapke GP_LMM	Hapke GSU
Al-Ca	47.59	48.26	8.92	29.16	0.83	0.65	9.08	57.28	9.07	29.16	1.98	1.38
Al-Fe	48.38	49.13	11.90	29.16	4.75	0.46	8.81	50.27	8.80	21.80	0.20	0.13
Al-Si	55.75	55.72	9.20	29.16	3.63	1.06	2.32	56.26	2.32	53.37	0.13	0.12
Al-Ti	54.64	54.80	9.38	19.73	2.57	0.08	3.74	55.35	3.73	29.13	0.15	0.03
Ca-Fe	47.88	48.47	11.34	29.16	4.59	1.13	9.22	50.65	9.21	29.16	0.44	0.40
Ca-Si	50.79	26.69	8.95	29.16	5.29	0.40	2.88	56.79	2.79	57.08	0.44	0.46
Ca-Ti	52.97	38.52	9.12	29.16	3.26	0.59	0.43	55.86	0.59	29.16	7.20	1.63
Fe-Si	49.97	50.25	11.08	28.61	4.11	1.48	6.75	51.39	6.75	29.49	0.15	0.05
Fe-Ti	50.22	50.44	10.49	20.79	4.90	0.57	6.80	52.12	6.79	29.16	0.85	0.41
Si-Ti	55.32	40.09	9.09	29.16	1.19	0.98	2.26	56.89	2.26	53.58	1.17	0.07

shown as well.

The outcomes of the experiments can be summarized as follows:

- The Fan model always fails and observes a pure mineral rather than a mixture.
- The Hapke model does not perform better than the linear model. Both models as well as geodesic unmixing generally perform poor on mixtures of minerals with large differences in grain size and/or density (e.g. Si-Ti).
- Overall, all three supervised methods outperform the unsupervised approaches and were able to accurately predict fractional abundances from almost all binary mixtures. The algorithms perform equally well for the spectrometer and the hyperspectral camera data.
- GP_LMM performs the best. The proposed method GSU is only slightly worse. In this single sensor experiment, the use of the geodesic abundance estimation step has no extra advantage.

3) *Experiment 3: Cross sensor unmixing:* In the third experiment, we investigated the performance of the supervised approaches in a cross sensor situation. For this, we trained the algorithms on the spectrometer data and applied the learned models on the camera data. Similarly, we trained the algorithms on the camera data and applied the learned models on the spectrometer data. We do not show the results of the unsupervised approaches, since they have been treated in the previous experiment.

Results are shown in Table V. The results clearly show the advantage of the proposed strategy to tackle the endmember variability. GSU outperforms the other methods in almost all cases. SM performs the worst, while GP_LMM that takes end-member variability partially into account, performs reasonably well on some mixtures but poor on others.

B. Experiments on RELAB dataset

1) *Experiment 4: Cross sensor experiment on simulated USGS and real Relab mineral mixtures:* From figure 5, we can observe that there is a large variability between the endmembers obtained from the USGS spectral library and the Relab dataset. The applied minerals have similar densities and grain sizes, well above the SWIR wavelength ranges, so that the Hapke model is expected to be efficient.

In the fourth experiment, we investigated the performance of the supervised approaches for predicting fractional abundances

of Relab mineral mixtures when the algorithms were trained on simulated mineral mixtures by the Hapke model on the USGS endmembers. For comparison, the results of the unsupervised approaches are shown as well.

In Table VI, we show the results. The Hapke model performs the best. All other unsupervised approaches perform poor. The Fan model fails. The geodesic unmixing approach and LMM produce similar results. From the supervised approaches, SM fails and GP_LMM performs poor on two of the four mixtures. Overall, GSU was able to predict fractional abundances of the Relab dataset accurately, sometimes even better than the Hapke model. This demonstrates the robustness of the proposed methodology with respect to endmember variability.

2) *Experiment 5: Cross sensor experiment on real USGS and Relab mineral data:* In the final experiment, we investigated the performance of the supervised approaches on Cal-Chl mixtures when trained on Relab spectra and tested on USGS spectra. Similarly, the algorithms were trained on USGS spectra and tested on Relab spectra. For comparison, the result of the unsupervised methods is shown as well.

Results are shown in Table VII. Except for the proposed approach, all methods including the Hapke model perform poor.

V. DISCUSSION

From the experiments, the following general conclusions can be drawn:

- In general, the LMM does not perform well on intimate mixtures of mineral powders. The good performance of the LMM for some binary mixture of the self-crafted dataset suggests that the nonlinearity in those datasets is not very complex. This might be due to the fact that some minerals in the mixtures have similar spectral behavior.
- The Fan model is not suitable for estimating fractional abundances of binary mixtures of mineral powders.
- In general, the Hapke model estimates the fractional abundances of the intimate mixtures reasonably well. As an exception, the Hapke model produced large errors on the binary mixtures of Calcite and Chlorite, Calcium and Titanium, and Silica and Titanium.
- Geodesic unmixing generally produces poor estimations. This is because the data manifold comprises a nonlinear

TABLE III: Estimated fractional abundances on the single sensor experiment (camera data).

Mixtures	Ground truth (first mineral)	LMM	Fan	Hapke	GU	SM	GP_LMM	GSU
Al-Si	0.593	0.437	0.012	0.473	0.290	0.503	0.543	0.496
	0.813	0.771	0.030	0.789	0.658	0.503	0.786	0.866
	0.929	0.918	0.036	0.926	0.837	0.503	0.890	0.959
Ca-Si	0.691	0.756	0.020	0.686	0.504	0.672	0.621	0.695
	0.871	0.837	0.027	0.803	0.822	0.907	0.882	0.921
	0.953	0.928	0.028	0.933	0.915	0.943	1.000	0.987
Ca-Ti	0.067	0.427	0.011	0.403	0.448	0.072	0.001	0.088
	0.177	0.667	0.021	0.626	0.759	0.173	0.180	0.226
	0.369	0.829	0.025	0.808	0.943	0.272	0.406	0.506
Fe-Al	0.525	0.485	0.917	0.356	0.712	0.446	0.536	0.527
	0.768	0.730	0.960	0.613	0.860	0.810	0.785	0.820
	0.901	0.886	0.984	0.824	0.906	0.910	0.896	0.944
Fe-Ca	0.418	0.515	0.916	0.361	0.611	0.485	0.501	0.483
	0.682	0.654	0.944	0.511	0.725	0.733	0.700	0.668
	0.865	0.858	0.978	0.779	0.887	0.838	0.887	0.889
Fe-Si	0.828	0.731	0.963	0.638	0.604	0.859	0.821	0.830
	0.935	0.932	0.999	0.910	0.951	0.921	0.942	0.994
	0.978	0.966	1.000	0.955	0.853	0.978	0.965	0.976
Si-Ti	0.011	0.082	0	0.088	0.320	0.016	0.019	0.004
	0.031	0.188	0	0.196	0.386	0.044	0.048	0.047
	0.087	0.554	0.007	0.572	0.502	0.113	0.108	0.124

TABLE IV: Estimated fractional abundances on the single sensor experiment (spectrometer data).

Mixtures	Ground truth (first mineral)	LMM	Fan	Hapke	GU	SM	GP_LMM	GSU
Al-Si	0.593	0.571	0.002	0.606	0.329	0.448	0.508	0.554
	0.813	0.965	0.023	0.970	0.635	0.702	0.768	0.853
	0.929	1.000	0.022	1.000	0.833	0.946	0.927	0.978
Ca-Si	0.691	0.662	0	0.451	0.511	0.662	0.628	0.622
	0.871	0.850	0.002	0.820	0.829	0.799	0.903	0.891
	0.953	0.951	0.006	0.936	0.919	0.958	0.952	0.958
Ca-Ti	0.067	0.437	0.011	0.288	0.389	0.053	0.085	0.084
	0.177	0.670	0.009	0.581	0.671	0.258	0.174	0.222
	0.369	0.876	0.019	0.766	0.835	0.392	0.351	0.580
Fe-Al	0.525	0.436	0.921	0.349	0.732	0.472	0.535	0.612
	0.768	0.671	0.954	0.595	0.888	0.494	0.768	0.833
	0.901	0.953	0.993	0.938	0.941	0.494	0.883	0.901
Fe-Ca	0.418	0.427	0.921	0.381	0.654	0.490	0.547	0.488
	0.682	0.627	0.950	0.564	0.755	0.665	0.690	0.675
	0.865	0.927	0.991	0.903	0.899	0.911	0.890	0.893
Fe-Si	0.828	0.707	0.972	0.662	0.681	0.844	0.833	0.820
	0.935	0.996	0.999	0.998	0.960	0.882	0.929	0.977
	0.978	1.000	1.000	1.000	0.877	0.966	0.974	0.958
Si-Ti	0.011	0.178	0	0.151	0.370	0.012	0.016	0.001
	0.031	0.225	0	0.219	0.404	0.021	0.028	0.010
	0.087	0.394	0.003	0.418	0.483	0.041	0.075	0.055

relationship between the arc length and the fractional abundances.

- Most of the supervised methods can estimate fractional abundances of test spectra accurately when trained on the same data manifold.
- In cross sensor situations, SM performs poor, since it cannot cope with endmember variability. In GP_LMM, the endmember variability is partially taken into account, by mapping the endmembers along with the mixtures, leading to improved results.
- The proposed approach GSU was found to be the most consistent and performed well for almost all mineral mixtures used in this study. This demonstrates the potential of the proposed methodology, in particular in cross sensor situations.

VI. CONCLUSION

In this work, we have proposed a strategy for nonlinear unmixing, taking into account spectral variability. The method contains a geodesic unmixing step that is invariant to end-member variability, and a supervised mapping step to learn the nonlinearity. The approach was validated and compared to a number of spectral mixing models and supervised unmixing approaches on binary mixtures of mineral powders, in single sensor and cross sensor situations. In future work, we will adapt the proposed method to be applicable on polynary mixtures.

APPENDIX

A nonlinear relationship exists between the arc length and the fractional abundances in data manifolds that are generated by nonlinear mixing models. As a result, the geodesic distance

TABLE V: Cross sensor results on self-crafted mineral mixtures.

Mixtures	Ground truth (first mineral)	HSI SM	HSI GP_LMM	HSI GSU	Spectrometer SM	Spectrometer GP_LMM	Spectrometer GSU
Al-Si	0.385	0.999	0.194	0.354	0.969	0.745	0.488
	0.593	0.956	0.266	0.536	0.973	0.885	0.638
	0.724	0.998	0.439	0.872	0.974	0.976	0.846
	0.813	0.992	0.538	0.655	0.974	0.979	0.856
	0.879	0.999	0.607	0.803	0.974	0.981	0.880
	0.929	0.992	0.664	0.700	0.974	0.966	0.916
	0.968	0.998	0.755	0.967	0.974	0.941	0.969
Ca-Si	0.494	0.394	0.521	0.440	0.319	0.422	0.513
	0.691	0.559	0.606	0.656	0.482	0.511	0.725
	0.802	0.675	0.660	0.728	0.790	0.633	0.820
	0.871	0.733	0.882	0.860	0.861	0.795	0.894
	0.919	0.822	0.918	0.901	0.896	0.812	0.934
	0.953	0.795	0.926	0.931	0.892	0.852	0.966
	0.979	0.877	0.940	0.933	0.887	0.849	0.990
Ca-Ti	0.030	0.061	0.005	0.031	0.018	0.025	0.030
	0.067	0.085	0.011	0.084	0.010	0.100	0.053
	0.115	0.084	0.020	0.123	0.020	0.166	0.100
	0.177	0.232	0.065	0.194	0.024	0.324	0.170
	0.265	0.170	0.093	0.297	0.047	0.400	0.249
	0.369	0.291	0.123	0.464	0.098	0.448	0.315
	0.599	0.278	0.130	0.604	0.200	0.463	0.607
Fe-Al	0.321	0.589	0.305	0.318	0.934	0.329	0.318
	0.525	0.666	0.486	0.537	0.390	0.546	0.520
	0.666	0.606	0.655	0.683	0.174	0.745	0.647
	0.768	0.647	0.729	0.757	0.433	0.857	0.790
	0.847	0.601	0.799	0.940	0.483	0.976	0.884
	0.901	0.605	0.807	0.834	0.725	0.974	0.890
	0.958	0.540	0.825	0.862	0.817	0.999	0.837
Fe-Ca	0.236	0.096	0.641	0.235	0.053	0.017	0.237
	0.418	0.297	0.763	0.433	0.105	0.269	0.413
	0.563	0.397	0.783	0.570	0.214	0.323	0.547
	0.682	0.619	0.840	0.687	0.481	0.504	0.675
	0.781	0.790	0.890	0.792	0.771	0.696	0.769
	0.865	0.808	0.921	0.867	0.760	0.838	0.863
	0.937	0.738	0.935	0.936	0.901	0.913	0.936
Fe-Si	0.674	0.226	0.613	0.673	0.483	0.735	0.679
	0.828	0.302	0.784	0.806	0.633	0.881	0.837
	0.897	0.215	0.879	0.893	0.714	0.936	0.920
	0.935	0.506	0.957	0.938	0.731	0.972	0.938
	0.960	0.469	0.946	0.962	0.798	0.973	0.951
	0.978	0.443	0.939	0.967	0.782	0.972	0.963
	0.990	0.240	0.918	0.939	0.873	0.962	0.955
Si-Ti	0.005	0.074	0.042	0.004	0.050	0.057	0.005
	0.011	0.046	0.066	0.008	0.045	0.024	0.020
	0.018	0.087	0.053	0.006	0.022	0.021	0.022
	0.031	0.184	0.143	0.030	0.009	0.012	0.036
	0.051	0.230	0.108	0.042	0.008	0.009	0.059
	0.087	0.210	0.265	0.105	0.008	0.020	0.083
	0.182	0.227	0.289	0.181	0.005	0.053	0.187

TABLE VI: Cross sensor results on real Relab mineral mixtures, where supervised approaches are trained on simulated USGS mixtures.

Minerals	Ground truth (first mineral)	LMM	Fan	Hapke	GU	SM	GP_LMM	GSU
Br-An	0.217	0.497	0.628	0.203	0.496	0.278	0.222	0.236
	0.454	0.739	0.823	0.461	0.737	0.040	0.424	0.492
	0.714	0.892	0.930	0.732	0.891	0.052	0.606	0.743
Ol-Br	0.248	0.118	0.068	0.236	0.131	0.971	0.416	0.265
	0.498	0.269	0.172	0.502	0.281	0.986	0.677	0.523
	0.748	0.500	0.369	0.772	0.505	0.991	0.931	0.771
An-Ol	0.288	0.163	0.034	0.315	0.175	0.0	0.184	0.235
	0.548	0.348	0.108	0.588	0.357	0.0	0.505	0.464
	0.784	0.575	0.261	0.811	0.579	0.0	0.798	0.699
Al-Qz	0.240	0.660	0.829	0.305	0.638	0.073	0.408	0.300
	0.486	0.794	0.890	0.488	0.772	0.025	0.670	0.544
	0.740	0.925	0.967	0.785	0.923	0.990	0.999	0.765

TABLE VII: Cross sensor results on real Relab mineral mixtures, where supervised approaches are trained on real USGS mixtures and vice-versa.

Minerals	Ground truth (first mineral)	LMM	Fan	Hapke	GU	SM	GP_LMM	GSU
Chl-Cal (USGS)	0.34 0.67	0.853 0.970	0.876 0.976	0.518 0.863	0.731 0.902	0.50 0.50	0.750 0.834	0.328 0.685
Chl-Cal (Relab)	0.258 0.510 0.758	0.718 0.849 0.973	0.819 0.905 0.982	0.491 0.696 0.986	0.710 0.834 0.945	0.492 0.496 0.497	0.897 0.947 0.931	0.334 0.520 0.817

between a mixture and an endmember does not provide the correct fractional abundance.

As an illustration, let us look at the Fan model in two dimensions. Consider a path in the spectral space from endmember $e_1 = \begin{bmatrix} 0.6 \\ 0.5 \end{bmatrix}$ to endmember $e_2 = \begin{bmatrix} 0.5 \\ 0.6 \end{bmatrix}$, parametrized by the fractional abundance of endmember e_2 ($t \in [0, 1]$). Then, according to the Fan model, each data point of the manifold can be described by the following equation:

$$y = \begin{bmatrix} 0.6 \\ 0.5 \end{bmatrix} (1-t) + \begin{bmatrix} 0.5 \\ 0.6 \end{bmatrix} t + \begin{bmatrix} 0.6 \\ 0.5 \end{bmatrix} \odot \begin{bmatrix} 0.5 \\ 0.6 \end{bmatrix} (1-t)t \quad (11)$$

The arc length (geodesic distance) between e_1 and the datapoint $y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$ (see Fig. 7 for the data manifold) can be determined as follows:

Fig. 7: Data manifold of the Fan model.

$$\begin{aligned} \text{Arc length}(t) &= \int_0^t \sqrt{\left(\frac{dy_1}{dt}\right)^2 + \left(\frac{dy_2}{dt}\right)^2} dt \\ &= \int_0^t \sqrt{(0.2 - 0.6t)^2 + (0.4 - 0.6t)^2} dt \\ &= 0.1(t - 0.5)\sqrt{18t^2 - 18t + 5} - 0.0117851 \\ &\quad \times \text{arcsinh}(3 - 6t) + 0.1332340 \end{aligned} \quad (12)$$

which is clearly nonlinearly related to t .

This nonlinear relationship is caused by the fact that the curvature(κ) of the manifold is not constant:

$$\begin{aligned} \kappa &= \frac{\left\| \frac{dy}{dt} \times \frac{d^2y}{dt^2} \right\|}{\left\| \frac{dy}{dt} \right\|^3} \\ &= \frac{0.12}{((0.2 - 0.6t)^2 + (0.4 - 0.6t)^2)^{3/2}} \end{aligned} \quad (13)$$

where $\times$ denotes the cross product between two vectors and $\|\cdot\|$ is the Euclidean norm of the vector.

ACKNOWLEDGEMENT

The research presented in this paper is funded by BELSPO (Belgian Science Policy Office) in the frame of the STEREO III programme – project GEOMIX (SR/06/357). The authors would like to thank the company Engie-Laborelec for the use of their hyperspectral SWIR camera, and Prof. R. Samson for the use of the spectrometer.

REFERENCES

- [1] N. Keshava and J. F. Mustard, "Spectral unmixing," *IEEE Signal Processing Magazine*, vol. 19, no. 1, pp. 44–57, Jan 2002.
- [2] J. W. Boardman, "Geometric mixture analysis of imaging spectrometry data," in *IEEE International Geoscience and Remote Sensing Symposium (IGARSS)*, vol. 4, Aug 1994, pp. 2369–2371.
- [3] D. C. Heinz and Chein-I-Chang, "Fully constrained least squares linear spectral mixture analysis method for material quantification in hyperspectral imagery," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 39, no. 3, pp. 529–545, 2001.
- [4] R. Heylen, M. Parente, and P. Gader, "A review of nonlinear hyperspectral unmixing methods," *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 7, no. 6, pp. 1844–1868, June 2014.
- [5] W. Fan, B. Hu, J. Miller, and M. Li, "Comparative study between a new nonlinear model and common linear model for analysing laboratory simulated-forest hyperspectral data," *International Journal of Remote Sensing*, vol. 30, no. 11, pp. 2951–2962, 2009.
- [6] R. Heylen and P. Scheunders, "A multilinear mixing model for nonlinear spectral unmixing," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 54, no. 1, pp. 240–251, Jan 2016.
- [7] A. Marinoni and P. Gamba, "A novel approach for efficient p -linear hyperspectral unmixing," *IEEE Journal of Selected Topics in Signal Processing*, vol. 9, no. 6, pp. 1156–1168, Sep. 2015.
- [8] A. Marinoni, J. Plaza, A. Plaza, and P. Gamba, "Nonlinear hyperspectral unmixing using nonlinearity order estimation and polytope decomposition," *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 8, no. 6, pp. 2644–2654, June 2015.
- [9] A. Marinoni, A. Plaza, and P. Gamba, "Harmonic mixture modeling for efficient nonlinear hyperspectral unmixing," *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 9, no. 9, pp. 4247–4256, Sep. 2016.
- [10] B. Hapke, R. Nelson, and W. Smythe, "The opposition effect of the moon: Coherent backscatter and shadow hiding," *Icarus*, vol. 133, no. 1, pp. 89 – 97, 1998.
- [11] B. Hapke, "Bidirectional reflectance spectroscopy: 1. theory," *Journal of Geophysical research*, vol. 86, pp. 3039–3054, 1981.

- [12] J. Chen, C. Richard, and P. Honeine, "Nonlinear unmixing of hyperspectral data based on a linear-mixture/nonlinear-fluctuation model," *IEEE Transactions on Signal Processing*, vol. 61, no. 2, pp. 480–492, 2013.
- [13] Y. Gu, S. Wang, and X. Jia, "Spectral unmixing in multiple-kernel hilbert space for hyperspectral imagery," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 51, no. 7, pp. 3968–3981, 2013.
- [14] J. Broadwater, R. Chellappa, A. Banerjee, and P. Burlina, "Kernel fully constrained least squares abundance estimates," in *2007 IEEE International Geoscience and Remote Sensing Symposium*, 2007, pp. 4041–4044.
- [15] J. Broadwater and A. Banerjee, "A comparison of kernel functions for intimate mixture models," in *2009 First Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing*, 2009, pp. 1–4.
- [16] G. Foody, "Relating the land-cover composition of mixed pixels to artificial neural network classification output," *Photogr. Eng. Remote Sens.*, vol. 62, no. 5, p. 491–499, 1996.
- [17] G. Foody, R. Lucas, P. Curran, and M. Honzak, "Non-linear mixture modeling without end-members using an artificial neural network," *Int. J. Remote Sens.*, vol. 18, no. 4, p. 937–953, 1997.
- [18] P. Atkinson, M. Cutler, and H. Lewis, "Mapping sub-pixel proportional land cover with avhrr imagery," *International Journal of Remote Sensing*, vol. 18, no. 4, pp. 917–935, 1997.
- [19] A. Okujeni, S. van der Linden, L. Tits, B. Somers, and P. Hostert, "Support vector regression and synthetically mixed training data for quantifying urban land cover," *Remote Sensing of Environment*, vol. 137, pp. 184 – 197, 2013.
- [20] G. Licciardi and F. D. Frate, "Pixel unmixing in hyperspectral data by means of neural networks," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 49, pp. 4163–4172, 2011.
- [21] B. Koirala, R. Heylen, and P. Scheunders, "A neural network method for nonlinear hyperspectral unmixing," in *IEEE Intern. Geosci Remote Sens. Symp.*, 2018, pp. 4233–4236.
- [22] B. Koirala, M. Khodadadzadeh, C. Contreras, Z. Zahiri, R. Gloaguen, and P. Scheunders, "A supervised method for nonlinear hyperspectral unmixing," *Remote Sensing*, vol. 11, no. 20, p. 2458, Oct 2019.
- [23] L. Drumetz, J. Chanussot, and C. Jutten, "Chapter 2.7 - variability of the endmembers in spectral unmixing," in *Hyperspectral Imaging*, ser. Data Handling in Science and Technology, J. M. Amigo, Ed. Elsevier, 2020, vol. 32, pp. 167 – 203.
- [24] A. Zare and K. C. Ho, "Endmember variability in hyperspectral analysis: Addressing spectral variability during spectral unmixing," *IEEE Signal Processing Magazine*, vol. 31, no. 1, pp. 95–104, 2014.
- [25] L. Drumetz, J. Chanussot, C. Jutten, W. Ma, and A. Iwasaki, "Spectral variability aware blind hyperspectral image unmixing based on convex geometry," *IEEE Transactions on Image Processing*, vol. 29, pp. 4568–4582, 2020.
- [26] L. Drumetz, B. Ehsandoust, J. Chanussot, B. Rivet, M. Babaie-Zadeh, and C. Jutten, "Relationships between nonlinear and space-variant linear models in hyperspectral image unmixing," *IEEE Signal Processing Letters*, vol. 24, no. 10, pp. 1567–1571, 2017.
- [27] A. Halimi, P. Honeine, and J. M. Bioucas-Dias, "Hyperspectral unmixing in presence of endmember variability, nonlinearity, or mismodeling effects," *IEEE Transactions on Image Processing*, vol. 25, no. 10, pp. 4565–4579, 2016.
- [28] A. Halimi, J. M. Bioucas-Dias, N. Dobigeon, G. S. Buller, and S. McLaughlin, "Fast hyperspectral unmixing in presence of nonlinearity or mismodeling effects," *IEEE Transactions on Computational Imaging*, vol. 3, no. 2, pp. 146–159, 2017.
- [29] W. Luo, L. Gao, R. Zhang, A. Marinoni, and B. Zhang, "Bilinear normal mixing model for spectral unmixing," *IET Image Processing*, vol. 13, no. 2, pp. 344–354, 2019.
- [30] Z. Wang, M. He, Z. Ye, K. Xu, Y. Nian, and B. Huang, "Reconstruction of hyperspectral images from spectral compressed sensing based on a multitype mixing model," *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 13, pp. 2304–2320, 2020.
- [31] R. Heylen, D. Burazerovic, and P. Scheunders, "Non-linear spectral unmixing by geodesic simplex volume maximization," *IEEE Journal of Selected Topics in Signal Processing*, vol. 5, no. 3, pp. 534–542, 2011.
- [32] M. Zhao, J. Chen, and Z. He, "A laboratory-created dataset with ground truth for hyperspectral unmixing evaluation," *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 12, no. 7, pp. 2170–2183, 2019.
- [33] J. F. Mustard and C. M. Pieters, "Quantitative abundance estimates from bidirectional reflectance measurements," *Journal of Geophysical Research: Solid Earth*, vol. 92, no. B4, pp. E617–E626, 1987.
- [34] E. W. Dijkstra, "A note on two problems in connexion with graphs," *NUMERISCHE MATHEMATIK*, vol. 1, no. 1, pp. 269–271, 1959.
- [35] C. Rasmussen and C. Williams, *Gaussian Processes for Machine Learning*. New York: The MIT Press, 2006.
- [36] J. F. Mustard and C. M. Pieters, "Photometric phase functions of common geologic minerals and applications to quantitative analysis of mineral mixture reflectance spectra," *Journal of Geophysical Research*, vol. 94, pp. 13 619–13 634, 1989.

Bikram Koirala received the B.S. degree in Geomatic Engineering from the Purbanchal University, Nepal, and the M.S. degree in Geomatic Engineering from the University of Stuttgart, Germany in 2011 and in 2016 respectively. In 2017, he joined Vision Lab, Department of Physics, the University of Antwerp as a Ph.D. researcher. He is a student IEEE member. His research interest includes machine learning and hyperspectral image processing.

Zohreh Zahiri received the bachelor degree in Civil Engineering from Shahid Ashrafi Esfahani University, Isfahan, Iran, and the M.S. degree in Architectural Conservation from the Isfahan University of Art in 2009 and in 2013 respectively. She received her Ph.D. degree in "Characterization of facade materials using close-range hyperspectral data" from University College Dublin (UCD), Department of Civil Engineering, Dublin, Ireland in 2018. She is currently a postdoctoral researcher at Vision Lab, Department of Physics, University of Antwerp. Her

research interests are the application of hyperspectral imaging in civil engineering and related areas as well as data analysis methods.

Alfredo Lamberti received his M.S degree in Aerospace Engineering and Astronautics from the University of Naples "Federico II" in Italy in 2011. He received a PhD in Engineering Sciences from the Vrije Universiteit Brussel in 2016 on the topic of novel processing technologies for Fiber Bragg grating sensors in composite materials. Further research work involves Post Doc positions at Vrije Universiteit Brussel and Ghent University, mostly related to integrity assessment methods for composite materials. Alfredo joined the NDT team of ENGIE Laborelec in January 2019. Besides a versatile activity in site inspections (UT, PA, ET), other activities involve research and development on NDT methods (Thermography, TFM, PA, Hyperspectral, X-Ray CT, etc) for advanced damage detection of materials and work on robotized NDT inspection for application in aerospace, energy or quality evaluation of materials produced with additive manufacturing.

Paul Scheunders (M'98) received the M.S. degree and the Ph.D. degree in physics, with work in the field of statistical mechanics, from the University of Antwerp, Antwerp, Belgium, in 1986 and 1990, respectively. In 1991, he became a research associate with the Vision Lab, Department of Physics, University of Antwerp, where he is currently a full professor. His current research interest includes remote sensing and hyperspectral image processing. He has published over 200 papers in international journals and proceedings in the field of image processing, pattern recognition, and remote sensing. Paul Scheunders is Associate Editor of the IEEE Transactions on Geoscience and Remote Sensing and has served as a program committee member in numerous international conferences. He is a senior member of the IEEE Geoscience and Remote Sensing Society.