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## Propagation of uncertainty in atmospheric parameters to hyperspectral unmixing

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## ABSTRACT

Atmospheric correction (AC) is important in pre-processing of airborne hyperspectral imagery. AC requires knowledge on the atmospheric state expressed by atmospheric condition parameters. Their values are affected by uncertainties that propagate to the application level. This study investigates the propagation of uncertainty from column water vapor (CWV) and aerosol optical depth (AOD) towards abundance maps obtained by means of spectral unmixing. Both Fully Constrained Least Squares (FCLS) and FCLS with Total Variation (FCLS-TV) are applied. We use five simulated datasets contaminated by various noise levels. Three datasets cover two spectral scenarios with different endmembers. A univariate and a bivariate analysis are carried out on CWV and AOD. The other two datasets are used to analyze the effect of surface albedo. The analysis identifies trends in performance degradation caused by the gradual shift in parameter values from their true value. The maximum achievable performance depends upon spectral characteristics of the datasets, noise level, and surface albedo. As expected, under noisy conditions FCLS-TV performs better than FCLS. Our research opens new perspectives for applications where estimation of reflectance is so far considered to be deterministic.

### 1. Introduction

Hyperspectral imaging sensors record the at sensor radiance reflected from a surface, for hundreds of narrow contiguous spectral bands. A recorded image can thus be seen as a three dimensional cube with two spatial dimensions and one spectral dimension. A pixel in such a cube usually covers an area comprising several endmembers. These mixed pixels are in contrast with pure pixels that cover a single endmember. The occurrence of mixed pixels is due to two main reasons: i) the spatial resolution of a hyperspectral sensor is relatively low, thus, several endmembers share the spatial extent of a pixel, and ii) the underlying surface is a mixture of several materials.

As important information about the scene might reside in mixed pixels, extraction of quantities of interest at the subpixel level is needed. Spectral unmixing is a popular extraction method at the subpixel level. It exploits spectral information to derive the endmembers in the scene, their spectral signatures, and their fractional abundances, i.e. areas occupied by each endmember in each pixel. For a comprehensive review of unmixing techniques, see Bioucas-Dias et al. (2012) and the references therein. In this study, we rely on the Linear Mixture Model (LMM) (Keshava, 2003). It expresses the observed spectrum of a pixel as a linear combination of the spectra of the endmembers weighted by

their fractional abundances.

Spectral unmixing using the recorded radiance is challenging in the presence of the Earth atmosphere. This is primarily because of the interaction of the surface reflected radiation with the atmospheric constituents while propagating along the path from the target surface to the sensor (Verhoef and Bach, 2003). The interaction generates two main atmospheric effects: absorption by atmospheric gases in particular water vapor and ozone and aerosols in the visible and near-infrared spectral range and scattering by aerosols and molecules (Lenoble, 1998). In addition, on the path of the beam to the sensor, reflection by the surrounding area of the target pixel and radiance backscattered by the atmosphere that did not interact with the surface distorts the at sensor radiance.

An Atmospheric Correction (AC) algorithm retrieves the surface reflectance from the at sensor radiance. AC algorithms can be divided into scene based empirical algorithms and algorithms based on radiative transfer modeling. We use the latter, as it is a mature approach for routine processing of hyperspectral image data (Gao et al., 2006).

In radiative transfer modeling, the target radiance can be derived assuming a plane-parallel geometry of the atmosphere, whereas the viewing and illumination geometry and total optical depth of the atmosphere are known. For a reliable estimate of reflectance, the

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concentration of the atmospheric scatters and absorbers, i.e. the optical parameters, should be available at the time of imaging. In this paper, we analyze the effect of uncertainty in estimations of atmospheric aerosol optical depth (AOD) and column water vapor (CWV). Both CWV and AOD are highly varying in space and time. Thus, they are estimated directly from satellite or airborne (remote) observations. With knowledge of CWV and AOD, transmission of radiation through the atmosphere can be simulated.

Estimation of CWV from at sensor radiance consists of identification of the measurement channels, identification of reference channels, and using a relation between reference and measurement channels (Carrere and Conel, 1993). These methods are limited with respect to several assumptions. First, surface reflectance is assumed to vary with wavelength in a linear way; second, the effect of sensor noise is often not considered, and third, uncertainty emerging from instrument characterization is ignored (Rodger, 2011; Qu et al., 2003).

Estimation of AOD consists of determining aerosol radiative properties characterized by their shape, their size, their chemical composition, and total amount (Diner et al., 2005). The MODIS science team (Remer et al., 2005) has developed the dense dark object method to estimate AOD that is further developed in Richter et al. (2006). The limitation of such methods is their suitability for pixels with dense vegetation. For scenes with dark pixels that are clustered at a few locations, pixelwise estimation of AOD is challenging. Besides, at sensor based inference of AOD is adversely affected by noise of at sensor radiance.

These assumptions and limitations, reasonable as they are, cause uncertainty in the estimation of CWV and AOD which likely propagates to reflectance estimates.

The objective of this paper is to analyze the impact of uncertainty in unmixing caused by CWV and AOD, given their specific influence on the estimated reflectance spectra. A basic hypothesis of unmixing is that the estimated reflectance spectra are free from atmospheric artefacts. By ignoring uncertainty in the AC parameters, however, it is likely that this hypothesis is violated. The paper specifically focuses on an operational processing chain. The operational processing chain is implemented in the multi-mission Processing, Archiving, and distribution Facility (PAF) for Earth observation products (Richter, 2007). Experiments in this paper are performed using the PAF incorporated in the Central Data Processing Center (CDPC) (Biesemans et al., 2007) at the Flemish Institute for Technological Research.

## 2. Theoretical background

### 2.1. Basic atmospheric effect modeling

The fraction ( $\rho_t$ ) of the total irradiance at the surface ( $E_g$ ) reflected by the earth surface depends upon the type of surface, illumination ( $\theta_s$ ), viewing geometry ( $\theta_v$ ), and wavelength ( $\lambda$ ). On the path of the beam to the sensor other radiation components are added to the radiance reflected by the surface ( $L_t(\lambda)$ ) due to atmospheric scattering. We distinguish four contributions to the at sensor radiance ( $L_{rs,t}(\lambda)$ ):

$$L_{rs,t}(\lambda) = L_t(\lambda) + L_{pa}(\lambda) + L_{pb}(\lambda) + L_b(\lambda). \quad (1)$$

$L_t(\lambda)$  contains the target surface information,  $L_{pa}(\lambda)$  and  $L_{pb}(\lambda)$  are path radiance and background path radiance, respectively, that enter the IFOV of the sensor due to scattering, and  $L_b(\lambda)$  is the background radiance, or adjacency effect, being the average radiance of the surrounding surface.

For a target surface with reflectance  $\rho_t(\lambda)$  and background reflectance  $\rho_{bck}(\lambda)$ , the background path radiance, background radiance, and target radiance are:

$$L_{pb}(\lambda) = \frac{1}{\pi} \rho_{bck}(\lambda) T_{dir}^+(\tau, \theta_v, \lambda) E_g(\lambda), \quad (2)$$

$$L_b(\lambda) = \frac{1}{\pi} \rho_{bck}(\lambda) T_{dir}^+(\tau, \theta_v, \lambda) E_g(\lambda), \quad (3)$$

$$L_t(\lambda) = \frac{1}{\pi} \rho_t(\lambda) T_{dir}^+(\tau, \theta_v, \lambda) E_g(\lambda), \quad (4)$$

where  $T_{tot}^+$  expresses the total upward transmittance, which is further subdivided in direct transmittance ( $T_{dir}^+$ ) and diffuse transmittance (Haan and Kokke, 1996). Let the residual terms in Eq. (1) be denoted by:

$$L_{rs,b}(\lambda) = L_{pa}(\lambda) + L_{pb}(\lambda) + L_b(\lambda). \quad (5)$$

Then the background reflectance can be retrieved using

$$\rho_{bck}(\lambda) = \frac{L_{rs,b}(\lambda) - L_{pa}(\lambda)}{C} \quad (6)$$

with

$$C = \cos(\theta_s) T_{tot}^+(\tau, \theta_v, \lambda) T_{tot}^-(\theta_s, \lambda) F + S [L_{rs,b}(\lambda) - L_{pa}(\lambda)]$$

where  $S$  is the spherical albedo for illumination from below of the atmosphere and  $T_{tot}^-$  expresses the total downward transmittance. Substituting the expression for  $\rho_{bck}(\lambda)$ , the target reflectance equals

$$\rho_t(\lambda) = \frac{L_{rs,t}(\lambda) - L_{pa}(\lambda) + [L_{rs,t}(\lambda) - L_{rs,b}(\lambda)] T_{dir}^+(\tau, \theta_v, \lambda) T_{diff}^+(\tau, \theta_v, \lambda)}{C}. \quad (7)$$

The basic atmospheric effect model is well described in Gao et al. (2009). We use MODTRAN 4 (Berk et al., 2000) to estimate the radiance components in Eq. (7). It computes absorption and scattering in the terrestrial atmosphere at high spectral resolution and is treated below as a black box. It allows one to pixelwise solving the DIScrete Ordinate Radiative Transfer (DISORT) (Stamnes et al., 1988) for accurate computations of atmospheric multiple scattering. In an operational processing chain, however, the considerable execution time to do so is a problem. Therefore, MODTRAN 4 is executed for a uniform Lambertian surface reflectance with a spectrally flat surface albedo of  $A_{pp} = 0$ ,  $A_{pp} = 0.5$ , and  $A_{pp} = 1.0$ . In this way, the various radiance components for a given atmospheric state and angular geometry are determined. This is the MODTRAN interrogation technique that has been used in operational processing chains to derive the same radiance component as in Eq. (7) (Verhoef and Bach, 2003; Sterckx et al., 2016). MODTRAN 4 provides four radiance components:

1. The total radiance as measured by the sensor,  $L_{rs,t}(\lambda)$ ,
2. The total path radiance  $L_{path}(\lambda)$  that consists of the light scattered in the path,
3. The total ground radiance that consists of all the light reflected by the surface and traveling directly towards the sensor,  $L_{gnd}(\lambda)$ ,
4. The direct ground reflectance,  $L_{dir}(\lambda)$  as a fraction of  $L_{gnd}(\lambda)$  resulting from direct illumination of the ground surface.

The four components are then combined using Eq. (7).

### 2.2. The linear mixture model (LMM) and unmixing methods

Let  $y \in \mathbb{R}^B$  be the reflectance spectrum of one pixel, where  $B$  is the number of spectral bands. According to the LMM, it can be expressed as a linear combination of the spectra of the endmembers, weighted by their fractional abundances:

$$y = A \cdot x + n. \quad (8)$$

Here,  $A \in \mathbb{R}^{B \times m}$  is the set of endmembers in the scene serving as a spectral library containing  $m$  pure spectra,  $x \in \mathbb{R}^m$  is the vector of corresponding fractional abundances compatible with  $A$ , and  $n \in \mathbb{R}^B$  is a noise vector. In this paper, we assume that  $A$  is available a priori. Unmixing thus aims at identifying the atoms of  $A$  which are active in each pixel and their respective abundances. To solve Eq. (8), we

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