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Nonlinear Hyperspectral Mixture Analysis for tree cover estimates in orchards

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ABSTRACT

Accurate monitoring of spatial and temporal variation in tree cover provides essential information for steering management practices in orchards. In this light, the present study investigates the potential of Hyperspectral Mixture Analysis. Specific focus lies on a thorough study of non-linear mixing effects caused by multiple photon scattering. In a series of experiments the importance of multiple scattering is demonstrated while a novel conceptual Nonlinear Spectral Mixture Analysis approach is presented and successfully tested on in situ measured mixed pixels in *Citrus sinensis* L. orchards. The rationale behind the approach is the redistribution of nonlinear fractions (i.e., virtual fractions) among the actual physical ground cover entities (e.g., tree, soil). These 'virtual' fractions, which account for the extent and nature of multiple photon scattering only have a physical meaning at the spectral level but cannot be interpreted as an actual physical part of the ground cover. Results illustrate that the effect of multiple scattering on Spectral Mixture Analysis is significant as the linear approach provides a mean relative root mean square error (RMSE) for tree cover fraction estimates of 27%. While traditional nonlinear approaches only slightly reduce this error (RMSE = 23%), important improvements are obtained for the novel Nonlinear Spectral Mixture Analysis approach (RMSE = 12%).

1. Introduction

In agricultural perennial plant production systems, such as orchards, information on spatial and temporal variation in vegetation cover has proven useful for steering management practices (Fitzgerald et al., 2005; Fares et al., 2008; Peddle & Smith, 2005). Tree canopy cover, which is highly correlated with leaf area index and biomass (Fitzgerald et al., 2005; Peddle & Smith, 2005), governs radiation interception and affects orchard yield potential and crop water requirements (Lelong et al., 1998). As such, it influences pest and disease management (Goodwin et al., 2005; Muhammed & Larsolle, 2003). Large variations in tree cover can lead to inefficient use of resources (e.g., pesticides, fertilizer, water, labor), thus posing risks to the production potential (e.g., water stress, nutrient deficiency) and the environment (e.g., excess runoff, salinity, soil nitrification and acidification) (Castro et al., 2006; Fares et al., 2008). A robust and accurate technique for site specific monitoring of tree cover in orchards would therefore result in important ecological and economic benefits.

Remote sensing has considerable potential for providing accurate estimates of orchard tree cover as an alternative to labor intensive and expensive field measurements. Space-borne spectral sensors allow for frequent and relatively inexpensive monitoring over large areas. For monitoring and mapping purposes Spectral Mixture Analysis (SMA) is an often used image analysis technique (e.g., Adams et al., 1993; Goodwin et al., 2005; Lelong et al., 1998; Muhammed & Larsolle, 2003; Peddle & Smith, 2005; Settle & Drake, 1993). SMA provides sub-pixel cover distribution maps. The technique is preferred over traditional pixel-based image classification as it accounts for the undesired spectral contribution of background features (e.g., soils, weeds) which are prevalent in agricultural scenes (Fitzgerald et al., 2005; Lelong et al., 1998).

Conventional SMA approaches model a mixed spectrum as a linear combination of pure spectral signatures of its constituent components (i.e., endmembers), weighted by their sub-pixel fractional cover (i.e., Linear Spectral Mixture Model, LSMM) (e.g., Adams et al., 1993; Settle & Drake, 1993). Once a set of appropriate endmembers and their corresponding spectral signatures have been defined, sub-pixel cover distribution maps can be generated by model inversion using approaches such as Singular Value Decomposition (Asner & Lobell, 2000), Gramm–Schmidt Orthogonalization (Adams et al., 1995), maximum-likelihood (Settle, 2006) or least-squares error (LSE) analysis (Barducci & Mecocci, 2005).

SMA retrieved cover fraction estimates are frequently altered by non-instrumentally induced errors. Errors can be injected into cover fractions because of (i) the lack of ability of SMA techniques to account for endmember variability, caused by spatial and temporal changes in (bio)physical and (bio)chemical conditions of the different land cover types (i.e., crop, soil, weed) (e.g., Roberts et al., 1998; Sabol et al., 1992); and (ii) the multiple scattering of photons between different

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surface components, which violates the linearity assumption of mixture models (Borel & Gerstl, 1994; Roberts, 1991). Over the past decades SMA studies have focused on solving the endmember variability problem, neglecting the effects of multiple scattering and the resulting nonlinear mixing. As a result, contrary to nonlinear mixing techniques numerous solutions are available to account for endmember variability based on iterative mixture analysis cycles (e.g., Asner & Lobell, 2000; Bateson et al., 2000; Roberts et al., 1998; Rogge et al., 2006), waveband selection algorithms (e.g., Asner & Lobell, 2000; Somers et al., in press) and spectral normalization techniques (e.g., Asner & Lobell, 2000; Li, 2004; Wu, 2004; Zhang et al., 2004, 2005). Nonlinear mixing due to multiple scattering of photons has been firmly established for mineral soils (Mustard & Pieters, 1987), and water (Mertes et al., 1993) and has widely been reported in plant–soil mixtures (e.g., Borel & Gerstl, 1994; Huete, 1986; Roberts, 1991; Roberts et al., 1993; Ray & Murray, 1996). Nevertheless, in the majority of vegetation monitoring studies the effect of multiple scattering is neglected. LSMMs are still applied using arguments on the complex nature of multiple scattering and the simplicity and relative accuracy of the linear models (e.g., Fitzgerald et al., 2005; Tompkins et al., 1997). Asner and Lobell (2000) tried to diminish the effects of nonlinear mixing by only including SWIR2 (2050–2500 nm) spectral information in their LSMM. The rationale was that multiple scattering in vegetated areas is dominant in the NIR spectral domain (750–1450 nm) due to the near-lambertian scattering behavior of leaves in this part of the electromagnetic spectrum (Asner, 1998; Lobell et al., 2002), while it was less pronounced in the SWIR2 domain. Others circumvent the problem of nonlinear mixing by validating algorithms using synthetic imagery in which nonlinear mixing effects are excluded (e.g., Rogge et al., 2006; Somers et al., 2009a,b, in press). As a result, only limited focus has been given to Nonlinear Spectral Mixture Analysis (NSMA) in the literature.

Borel and Gerstl (1994) were one of the first to model the phenomenon of multiple scattering in plant–soil mixtures. Using a radiosity method, they illustrated that by including additional endmembers, each accounting for a characteristic interaction among ground objects, nonlinear spectral mixing could be accurately and realistically modeled. Although the approach has shown improved accuracies over Linear Spectral Mixture Analysis (LSMA) in both arid ecosystems (Ray & Murray, 1996) as well as in forest/grassland ecotones (Arai, 2007; Chen & Vierling, 2006), its validation has not yet been fully addressed.

Despite the numerous applications for SMA, nonlinearity has barely been investigated and the corresponding nonlinear mixing models have never been validated in agricultural production systems. Yet in agricultural fields and more specifically in orchards, plants are geometrically ordered which not only make these drastically different from the abovementioned environments but furthermore provides novel opportunities for consistent modeling of nonlinearity. Recall that multiple scattering is mainly determined by the 3D structure composition of the surrounding area. The presence of trees in relatively high densities, as observed in orchards, as such reinforces the occurrence of nonlinear mixing (Borel & Gerstl, 1994; Zhang et al., 2007). In sparsely vegetated arid regions, LSMMs tend to work well because plants are widely separated and thus the area of scattering is well localized covering a small area (Elmore et al., 2000; McGwire et al., 1999). As shown by Ray and Murray (1996), fractions in the close proximity of the plants are erroneous, but the error declines rapidly with increasing distance to the plant. The vertical structure of the canopy and the spatial distribution of the plants play an important role in nonlinearity, but also the leaf radiation transmittance. Relatively opaque leaves, such as conifer needles, tend to produce less NIR scattering than the relatively thin leaves of broadleaf plants and grasses observed in agricultural fields and orchards (Asner, 1998; Roberts et al., 2004). Thus, nonlinear mixing tends to be less significant in conifer ecosystems than in crop lands (Painter et al., 1998). All these considerations imply that orchards are splendid study objects for increased nonlinear mixing. Moreover, due to the spatial repetition of tree rows (i.e., fixed plant distances) and the consistency in tree structure (i.e., controlled by pruning) a mathematical description of nonlinear mixing seems feasible. Therefore, a thorough nonlinear model calibration, optimization and validation could have important positive repercussions for the use of SMA in orchards.

Hence, the present study aims at improved sub-pixel tree cover fraction estimates in plant production systems using SMA. A specific focus of this study is on a study of non-linear mixing effects. Citrus (*Citrus sinensis* L.) orchards are chosen as pilot plant production system. The research objectives can be summarized as follows:

(i) quantify the amplitude and nature of multiple scattering in orchards;
(ii) validate and optimize the performance of existing NLMMs in orchards (Chen & Vierling, 2006; Ray & Murray, 1996);
(iii) present an alternative NSMA approach for improved tree cover mapping in orchards.

In situ measured mixed pixel spectra (i.e., ground plots) and the corresponding pure sub-pixel endmember spectra of different endmember combinations in *Citrus* orchards were used for validation. Unlike imagery-based studies, controlled in situ measurements allow the use of pixel- or plot-specific reference endmembers to minimize the effects of endmember variability and to isolate the effect of multiple scattering (Ray & Murray, 1996).

2. Theoretical background

2.1. Linear Spectral Mixture Analysis

The physical assumption underlying Linear Spectral Mixture modeling is that each incident photon interacts with one earth surface component only and that the reflected spectra do not mix before entering the sensor (Adams et al., 1993; Settle & Drake, 1993). In its general form the LSMM can, as such, be described as:

$$R_i = \sum_{j=1}^{m} \left(f_j R_{i,j}\right) + \varepsilon_i \text{ with} \sum_{j=1}^{m} f_j = 1 \text{ and } 0 \le f_j \le 1 \qquad (1)$$

where R_i is the measured reflectance of a mixed pixel in spectral band i, $R_{i,j}$, the jth endmember reflectance for spectral band i. m is the number of endmembers and f_j is the sub-pixel cover fraction of the jth endmember in the pixel. The residual term ε_i is the unmodeled portion of the spectrum. The coefficients in Eq. (1) are often constrained to (i) sum to one and (ii) to be non-negative in order to obtain physically interpretable cover fraction estimates (Adams et al., 1993; Settle & Drake, 1993). Fraction estimates are obtained by inverting the model in Eq. (1). One possible solution is the LSE estimator which solves vector f such that the following equation is minimized:

$$\sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(\sum_{j=1}^{m} \left(f_j R_{i,j}\right) - R_i\right)^2. \qquad (2)$$

In Eq. (2) n is the number of available spectral bands. Agricultural fields are characterized by a limited number of well-defined land cover classes or endmembers being crop (i.e., tree) ($R_{i,t}$), weed ($R_{i,w}$), soil ($R_{i,s}$) and shade ($R_{i,sh}$) (Peddle & Smith, 2005).

2.2. Nonlinear Spectral Mixture Analysis

Traditionally, Nonlinear Spectral Mixture Models (NLMM) account for the presence of multiple photon interactions by introducing additional 'interaction' terms in LSMM (Eq. (1)). Each term accounts for multiple interactions between endmembers and is represented by the cross-product of the interacting endmembers (Borel & Gerstl,