The impact of atmospheric conditions and instrument noise on atmospheric correction and spectral mixture analysis of multispectral imagery

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ABSTRACT

The purpose of this study was to evaluate the effect of instrument noise, atmospheric conditions, and reflectance retrieval method on multispectral reflectance and fractional cover estimates derived from spectral mixture analysis. Top-of-atmosphere (TOA) radiance was simulated for pixels with various ground (fractional cover of green vegetation (GV), nonphotosynthetic vegetation (NPV), and soil) and atmospheric/geometric (solar zenith angle, visibility, and water vapor) conditions for four operational spaceborne multispectral images, Landsat 5 Thematic Mapper (TM), Landsat 7 Enhance Thematic Mapper Plus (ETM+), Landsat 8 Operational Land Imager (OLI), and the Moderate Resolution Imaging Spectroradiometer (MODIS). Instrument noise was added to the TOA radiance. Three reflectance retrieval methods were used to estimate surface reflectance, and fractional cover estimates of GV, NPV, and soil

were made using spectral mixture analysis (SMA) and multiple endmember spectral mixture analysis (MESMA). Among atmospheric characteristics, we found that visibility and solar zenith angle made the greatest contributions to spectral and fractional cover error. In all cases, GV fraction was estimated with lower error than NPV or soil fraction. The reflectance retrieval method that provided the best reflectance estimates did not produce the fractional cover estimates with the lowest error due to variable bias across bands. Fractional cover estimates for all ground components were strongly impacted by instrument noise, but MESMA significantly improved fractional cover estimates for NPV and soil, regardless of noise level. This study suggests that there are practical constraints on the level of accuracy that can be attained in multispectral estimates of NPV and soil. A set of recommendation for the use of spectral unmixing of multispectral reflectance data is developed.

Keywords: Landsat, MODIS, Thematic Mapper (TM), Enhanced Thematic Mapper Plus (ETM+), Operational Land Imager (OLI), surface reflectance, visibility, spectral mixture analysis, MODTRAN, noise, atmospheric correction

INTRODUCTION

Multispectral remote sensing in the reflected solar spectrum has become a critical way that both the scientific and lay communities learn about the Earth's surface. However, there are limitations in the information about the surface that can be retrieved in the reflected solar spectrum. The fact that light from the sun must pass twice through the atmosphere imposes constraints on retrieval of the surface reflectance, particularly with multispectral instruments that do not have the spectral resolution to directly estimate atmospheric conditions (e.g., Gao and Goetz 1990; Green et al. 1993). The need to remove the effect of the atmosphere requires

selection of a reflectance retrieval method, which invariably impacts the accuracy of surface reflectance estimates (e.g., Moran et al. 1992).

Instrument noise can also influence the utility of remote sensing data (e.g., Drake et al. 1999). There are several types of instrument noise (e.g., dark-target vs. signal-dependent noise, coherent vs. incoherent noise), but these are commonly lumped together as the signal-to-noise ratio (SNR; e.g., Helder et al. 2004; Platt and Goetz 2004). Improvements in the SNR for multispectral data have significantly enhanced the precision of these data and increased their usefulness in remote sensing of the Earth surface (Mika 1997).

The purpose of this study is to investigate the impact of atmospheric conditions, reflectance retrieval method, and instrument noise on estimates of fractional cover derived from spectral mixture analysis (SMA). There are many ways that estimated surface reflectance from spaceborne multispectral instruments is used to derive information about the Earth's surface. One of the most common, is the use of vegetation indices such as the Normalized Difference Vegetation Index (NDVI) or its successor, the Enhanced Vegetation Index (EVI), both of which are produced as standard products for the Moderate Resolution Imaging Spectroradiometer (MODIS) (Huete et al. 2002). These indices are generally employed to derive information about green vegetation (GV) because they exploit the strong NIR to red contrast characteristic of characteristics of turgid, green leaves (Horler et al. 1983; Filella and Penuelas 1994)

GV is undoubtedly a critical component of the Earth's ecosystems, but it is not the only component. In many cases, it does not even comprise the majority of fractional cover nor do its dynamics always dominate the annual and interannual cycle (e.g., Okin 2010). Nonphotosynthetic vegetation (NPV) and soil in many systems dominate the surface reflectance. This is particularly true in drylands where there can be a significant fraction of soil and NPV

cover year-round (Okin et al. 2015), but many more humid environments also exhibit periods of high soil and NPV cover, such as wintertime deciduous forests. Tropical rainforests, even, can exhibit high NPV cover (e.g., Higgins et al. 2014).

SMA of some sort has proven the best, and maybe only, approach for simultaneous retrieval of GV, NPV, and soil fractional cover from relatively coarse-scale spaceborne multispectral data (e.g., Elmore et al. 2000; Asner and Heidebrecht 2002; Okin 2007; Guerschman et al. 2009; Yang et al. 2012; Quintano et al. 2013). But, the challenge of extracting NPV and soil information from multispectral images is augmented by the fact that their respective spectra are very similar (Okin 2007) and without data in the SWIR, they can be inseparable, although in contiguous spectra, they can be separated (e.g., Roberts et al. 1993 ; Asner and Lobell 2000). The difficulty of separating NPV and soil under the best of circumstances suggests that potential errors due to instrument noise, atmospheric factors, and reflectance retrieval may reduce our ability to extract full information about the Earth's land surface in terms of these ground components. This study is aimed at determining the error in fractional cover estimates arising from these factors.

METHODS

Top-of-atmosphere (TOA) radiance was simulated for four multispectral satellite remote sensing instruments (Landsat 5 TM, Landsat 7 ETM+, Landsat 8 OLI, and MODIS), then several methods were used to estimate surface reflectance from TOA radiance, and finally multiple endmember spectral mixture analysis (MESMA) was used to estimate the (known) fractional contribution of GV, NPV, and soil (Figure 1). Under normal remote sensing application conditions these fractional contributions would be interpreted as fractional cover of these ground

components. Hereafter and for the sake of simplicity, fractional contributions estimated by spectral unmixing will be referred to as fractional cover.

Simulation of TOA radiance

To simulate TOA radiance, first spectral surface reflectance, ρ_a , had to be established. ρ_a was estimated as the linear mixture of endmember spectra of GV, NPV, and soil:

$$\rho_{a,i} = f_{GV}\rho_{GV} + f_{NPV}\rho_{NPV} + f_{soil}\rho_{soil} \quad (1)$$

where f_i is the fractional cover of each endmember spectrum, ρ_i , and i is either GV, NPV, or soil. Three spectra each of f_i were used (Figure 2), resulting in 27 possible combinations of spectra. To control for difference in endmember brightness, which although real, potentially overlaps with other errors in reflectance inversion, all endmember spectra were set to a fixed reflectance (0.53) at a specific wavelength (1070 nm for GV, 1756 nm for NPV and soil). The reflectance value chosen was arbitrary; it was the actual reflectance of one of the measured field NPV spectra at 1756 nm, but the wavelengths for normalization were chosen to be near the maximum reflectance for all spectra for each cover type. The original field spectra were derived from contact-probe spectroscopy in the Kalahari (Meyer and Okin 2015). After adjusting for brightness, all endmember spectra were convolved to instrument wavebands. Instrument relative spectral response functions were obtained from the Landsat Spectral Characteristics Viewer (http://landsat.usgs.gov/tools_spectralViewer.php), which also includes MODIS relative spectral response functions.

All combinations of f_{GV} and f_{NPV} belonging to [0.01, 0.02, 0.05, 0.10, 0.20, 0.49] were used, with f_{soil} set to the value that makes all fractions sum to one, resulting in 36 mixtures. This scheme resulted in a total of 972 total reflectance spectra. Shade was not included.

Radiative transfer through the atmosphere has been well understood for decades (e.g., Chandrasekhar 1960). Here, MODTRAN 5 was used to simulate radiance (L_{TOA} in $\text{W m}^{-2} \text{sr}^{-2}$) for each instrument band at the top of the atmosphere using:

$$L_{TOA}(v, w, z, \rho, \lambda) = L_G(v, w, z, \rho, \lambda) + L_P(v, w, z, \rho, \lambda) \quad (2)$$

where v is the surface visibility (km), w is the column water vapor content of the atmosphere (g cm^{-2}), z is the solar zenith angle (degrees), λ is the instrument band, L_G is the solar radiance reflected from the surface and transmitted through the atmosphere and L_P is solar radiance reflected from the atmosphere. A mid-latitude summer atmosphere model was used, ozone column scaling was set to one, the CO_2 mixing ratio was 330 ppmv, and a rural aerosol model was used. Although 330 ppmv CO_2 is about 18% lower than present CO_2 (~400 ppmv), this difference in concentration is not expected to influence our results in any way since the bands of these multispectral sensors are chosen to avoid absorption bands of atmospheric gasses such as CO_2 . Atmospheric multiple scattering was calculated using an 8-stream DISORT algorithm with azimuthal dependence. Surface reflectance was assumed to be independent of solar or view angles. Latitude was set to 35°N (longitude: 0°) and time of day was set to 10:30 UTC to coincide approximately with the observation time of the Landsat and MODIS-Terra instruments. Other relevant geometric and atmospheric characteristics are given in Table 1. All combinations of these parameters were used, resulting in 27 model atmospheres.

Including atmospheric multiple scattering in our MODTRAN modeling approach resulted in values of L_G and L_P that were dependent upon surface reflectance. Therefore, in practice, L_G and L_P were simulated in MODTRAN for each model atmosphere (and solar geometry) for surfaces of constant reflectance at five reflectance levels (0.0, 0.25, 0.5, 0.75. and 1.0). For each

instrument band and each combination of z , w , and v , fourth-order polynomials were used to fit L_G and L_P to surface reflectance. Standard error for these fits was always < 0.0001 . For a given surface spectral reflectance, L_G and L_P were then estimated using these polynomial equations and L_{TOA} was estimated finally using Equation (2).

Addition of noise to TOA spectra and estimation of apparent surface reflectance

Once TOA radiance was estimated, signal-dependent noise was added to the radiance using:

$$L_{TOA, Noisy} = L_{TOA} (1 + 0.5 N(0,1) / \text{SNR}), \quad (3)$$

where $N(0,1)$ is a normal distribution with a mean of zero and a standard deviation of one, and SNR is the signal-to-noise ratio of a satellite sensor (Okin et al. 2001). For each model atmosphere ($n=36$) and surface spectrum ($n=972$), a noisy TOA spectrum was simulated 100 times. Satellite SNRs used in this study are given in Table 2. MODIS SNR was obtained from MODIS band specifications (<http://modis.gsfc.nasa.gov/about/specifications.php>). Landsat 7 ETM+ and Landsat 8 OLI SNR were obtained from the Landsat Data Continuity Mission (http://ldcm.nasa.gov/spacecraft_instruments/oli_perf.html). Landsat 5 TM was estimated from information in Helder et al. (2004) assuming a surface reflectance of 50% at $z = 42.2^\circ$. The use of SNR as the only metric of noise does not fully characterize instrument noise and does not allow dark-target (signal-independent) or other types of noise. However, 1) it is a common way to simply characterize instrument noise, 2) it is consistent with previous approaches (e.g., Okin et al. 2001; Platt and Goetz 2004), 3) it does represent relative differences in noise among the instruments used here (TM > ETM+ > MODIS > OLI) and 4) it is often the only noise information available for an instrument and it is the only noise information available for all of

the instruments considered here. Thus, for the purposes here, we believe that the use of SNR as the sole metric of instrument noise is an acceptable approach.

Estimation of surface reflectance from TOA radiance

Once noisy TOA radiance was simulated, surface reflectance was estimated using three common reflectance retrieval methods, followed by an additional correction to the reflectance from each of those methods resulting in six different apparent surface reflectance estimates for each noisy TOA radiance spectrum.

The first method was simple TOA reflectance, ρ_{TOA} , in which reflectance is estimated as:

$$\rho_{TOA} = \pi L_{TOA} / (\cos(z) L_{Sun}) \quad (4)$$

where L_{Sun} is the band-integrated TOA solar radiance (W m^{-2}) (NASA 2012). For each band L_{Sun} was calculated for each instrument band using the Second Simulation of a Satellite Signal in the Solar Spectrum (6S) radiative transfer code available at: 6s.ltdri.org (Kotchenova and Vermote 2007).

The second method was TOA reflectance with a dark-target correction, ρ_{DT} , in which reflectance is estimated as:

$$\rho_{TOA,DT} = \pi (L_{TOA} - L_{DT}) / (\cos(z) L_{Sun}) \quad (5)$$

where L_{DT} was calculated for each band using the MODTRAN-based approach described above assuming a surface reflectance of zero (Chavez 1988). Although in reality, L_{DT} would also have instrument noise, a single (modeled) value of L_{DT} was used so as not to inflate the number of cases to be considered and because path radiance is much smaller than total TOA radiance, thus the added noise due to L_{DT} would be small.

178 Third, we used a modification of the approach used for Landsat (Masek et al. 2008) and
 179 MODIS (Vermote and Kotchenova 2008) that employs the 6S atmospheric radiative transfer
 180 code. This approach estimates ρ_{TOA} as:

$$181 \quad \rho_{TOA} = T_{Gas} \rho_{Scatt} + T_{Scatt} T_{Water} \frac{\rho_{Surf}}{1 - S_{Scatt} \rho_{Surf}} \quad (6)$$

182 where ρ_{TOA} can be estimated from Equation (4), T_{Gas} is the transmissivity of the atmosphere due
 183 to gaseous absorption, ρ_{Scatt} is the reflectance of the atmosphere due to scattering by gasses and
 184 aerosols, T_{Scatt} is the transmission of the atmosphere due to scattering by gasses and aerosols, T_W
 185 is the transmission of the atmosphere due to water vapor, S_{Scatt} is the atmospheric spherical
 186 albedo due to scattering by gasses and aerosols, and ρ_{Surf} is the reflectance of the surface. Solving
 187 Equation (6) for ρ_{Surf} gives:

$$188 \quad \rho_{6S} = \rho_{Surf} = \frac{C}{CS_{Scatt} + 1}, \quad (7)$$

189 where,

$$190 \quad C = \frac{\frac{\rho_{TOA}}{T_{Gas}} - \rho_{Scatt}}{T_{Scatt} T_{Water}}. \quad (8)$$

191 The only modification made to this approach is that known atmospheric parameters (Table 1)
 192 were used to calculate atmospheric scattering, transmission, and spherical albedo from 6S. This
 193 eliminates estimation of atmospheric parameters as a source of error for the reflectance retrieval.

Most methods to determine surface reflectance result in some systematic atmosphere-dependent bias. To correct for this bias, reflectance estimated using Equations (4), (5), and (7) were corrected by applying a constant to each band that was equal to the average (known) reflectance used to produce the noisy TOA spectra divided by the average reflectance determined by one of the three reflectance inversion methods above. In practice, a spectrum for a known pseudo-invariant target is often used (e.g., Moran et al. 2001). However, use of a single pixel essentially encodes the error of that one pixel into the “improved” reflectance inversion for the whole image (Drake et al. 1999). The use of averages in our case obviates this problem, and with 972 spectra each simulated 100 times, we assume that the Gaussian noise in 97,200 spectra will cancel out resulting in a mostly noise-free average spectrum.

Spectral unmixing

Linear SMA was used to estimate fractional cover of GV, NPV, and soil from derived reflectance. In SMA, the apparent surface reflectance is assumed to be a linear combination of the reflectance of the spectra of the ground components, “endmembers”, weighted by their fractional cover in each simulated surface reflectance spectrum. The SMA equation for n endmembers is:

$$r_s = \sum_{k=1}^n f_k r_k + e, \quad (9)$$

where ρ_s is the apparent surface reflectance (ρ_{TOA} , $\rho_{TOA,DT}$, or ρ_{6S}), ρ_k is the reflectance of the k -th endmember, and f_k is the fractional cover of the k -th endmember (Shimabukuro and Smith 1991). The final term, ε , is the residual spectrum remaining after best-fit coefficients, f_k , have

214 been determined. Equation (9) is sometimes subject to the constraints that f_k must belong to the
 215 interval $[0,1]$ and/or

$$216 \quad \sum_{k=1}^n f_k = 1. \quad (10)$$

217 However, these were not enforced for this study because systematic biases in derived apparent
 218 surface reflectance caused them to increase fractional cover error. Here, 3-endmember models
 219 were used: GV, NPV, and soil. Our mixture models did not include shade as an endmember,
 220 consistent with the approach of Somers et al. (2009) and Asner and Heidebrecht (2003). Our
 221 approach is also consistent with that of Roberts et al. (1998; 2003) and Li et al. (2005) who
 222 report a shade fraction, but do not include it formally as an endmember and instead calculate it as
 223 $1 - \sum f_k$ after best-fit fractions have been determined through unmixing. Our approach differs from
 224 that of Elmore et al. (2000), who use a shade spectrum, derived from their TM imagery, as an
 225 endmember in the unmixing. This latter approach would be inappropriate inasmuch as spectrum
 226 fractions sum to one in the original ground reflectance, meaning that the original reflectance had
 227 no shade whatsoever.

228 MESMA is a version of SMA in which the best-fit coefficients of many different SMA
 229 models (a model is a unique combination of endmember spectra where each endmember belongs
 230 to a class such as GV, NPV, or soil) are calculated and the best model is picked among these
 231 (Roberts et al. 1998). One criterion often used in MESMA to pick the best model is *RMSE*:

$$232 \quad RMSE = \sqrt{\frac{1}{m} \sum_{b=1}^m (e_b)^2}, \quad (11)$$

where m is the number of bands; the model with the lowest $RMSE$ is chosen as the “best” model and the endmember fractions of this model are used as the best estimates of fractional ground cover (Roberts et al. 1998).

In practice, unmixing was done using linear least squares preceded by a Gram-Schmidt orthogonalization (Q-R decomposition) of the endmember matrix (Roberts et al. 1998). No constraints were placed on endmember fractions.

Three cases were considered.

- In Case 1, MESMA was used to unmix apparent surface reflectance and the original spectra used to create the TOA radiance (Figure 2) were used as endmembers. This is the least realistic of the cases considered here. It assumes perfect knowledge of ground spectra and no spectral variability outside that prescribed by endmember fractions. Error for this case thus cannot be related to endmember selection or unmixing method but is error resulting from the reflectance inversion alone.
- In Case 2, SMA using only the three average GV, NPV, and soil spectra (Figure 2) was used.
- In Case 3, MESMA using a new set of endmembers (Figure 3) was used, derived from the data of Meyer et al. (2015). The brightness of these endmembers was adjusted in a manner identical to the adjustment of the brightness of the original spectra. This case is the most realistic of those investigated here; it assumes no knowledge of the source reflectance spectra but does use spectra that were collected close in space and time to the source spectra. However, since the brightness of these endmembers was adjusted in a manner similar to those of the source reflectance endmembers, this case is still not entirely representative of most applications in which

there is no or little *a priori* knowledge about the actual ground spectra. Nonetheless, unmixing of spectra set to a known value at a specific wavelength is a useful approach to reduce the variability that is independent of spectral shape and has been used for unmixing approaches (e.g., Asner and Heidebrecht 2002).

Error Analysis

Several metrics were used to estimate error in both the retrieved apparent surface reflectance and the endmember fractions. In terms of the former, root mean squared error of the spectral reflectance ($RMSE_\rho$) was calculated as:

$$RMSE_r = \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{b=1}^m (r_{b,i,S} - r_{b,i,actual})^2 \quad (12)$$

where the subscript b refers to the m spectral bands for an instrument, the subscript i refers to the n number of modeled spectra, and ρ_S refers to the reflectance being evaluated. In addition, spectral mean error (ME_ρ) was calculated as:

$$ME_r = \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{b=1}^m (r_{b,i,S} - r_{b,i,actual}), \quad (13)$$

which is an estimate of the bias (across all bands) in the reflectance retrieval. $RMSE_\rho$ and ME_ρ can also be calculated for a single wavelength ($m = 1$).

In terms of error in endmember fractional cover, root-mean squared error in fraction cover ($RMSE_f$) was calculated as:

$$RMSE_f = \left(\frac{1}{n} \sum_{i=1}^n (f_{k,i}^{MESMA} - f_{k,i}^{actual})^2 \right)^{1/2}, \quad (14)$$

274 where $f_{k,i}^{MESMA}$ is the SMA- or MESMA-derived fractional cover of ground component k (GV,
 275 NPV, or soil), and $f_{k,i}^{actual}$ is actual fraction used to create the simulated spectrum. To characterize
 276 the bias in fraction retrieval, mean error of fractional cover (ME_f) was calculated as:

$$277 \quad ME_f = \frac{1}{n} \sum_{i=1}^n (f_{k,i}^{MESMA} - f_{k,i}^{actual}). \quad (15)$$

278 The term n in Equations (12) - (15) was either 972 or 97,200 depending on whether only the
 279 reflectance derived from non-noisy L_{TOA} was used (i.e., 972 different fractional
 280 cover/endmember combinations) or whether those derived from the noisy $L_{TOA, Noisy}$ was used
 281 (i.e., 100 noisy estimates of 972 fractional cover/endmember combinations), respectively.

282 This simulation approach allowed separation of different sources of error in endmember
 283 fractional cover estimates. Errors due solely to the surface reflectance inversion method
 284 (uncorrected and corrected) were determined for each ground cover type by calculating $RMSE_f$
 285 and ME_f from fractions calculated by Case 1 unmixing of the reflectance derived from the noise-
 286 free L_{TOA} . In this case, the effect of noise and endmember selection do not enter the calculation
 287 because the endmembers used for the unmixing are the same as those used to create L_{TOA} .
 288 Instrument noise should create variability in estimated endmember fractions. To assess this we
 289 calculated the standard deviation for each of the 972 fractional cover/endmember combinations
 290 of the fractions calculated using Case 1, and then averaged these across all 27
 291 geometric/atmospheric conditions. This provides an estimate of the average variability due solely
 292 to instrument noise for all geometric/atmospheric conditions examined here. Because Case 1
 293 unmixing was used, endmember selection again does not enter in as a source of error.

Errors due to the choice of endmembers (i.e. the unmixing Cases 2 and 3) were determined for each ground cover type by calculating $RMSE_f$ and ME_f from fractions calculated by unmixing the original surface reflectance spectra, ρ_{actual} . Since reflectance from noisy TOA radiance was not used, instrument noise does not enter the calculation. By definition (and also in practice), $RMSE_f$ and ME_f are zero for Case 1.

In addition, we examined the impact of geometric/atmospheric conditions (Table 1) on error, calculating multiple regressions of $RMSE_\rho$ and $RMSE_f$ across water vapor, visibility, and solar zenith angle. This analysis shows the extent to which the geometric and atmospheric conditions each impact fractional estimate errors. Because water vapor, visibility, and solar zenith angle have different orders of magnitude and ranges, we first transformed each of these variables to the range [0,1] by:

$$X \text{ (normalized)} = (X - X_{min}) / (X_{max} - X_{min}), \quad (16)$$

where X is either water vapor, visibility or solar zenith angle and min and max represent the minimum and maximum values in Table 1, respectively. This normalization allows direct comparison of the coefficients of regression because it forces the independent variables to the same scale.

RESULTS

Uncorrected derived apparent surface reflectance using all reflectance retrieval methods ($TOA = \rho_{TOA}$, $DT = \rho_{TOA,DT}$, $6S = \rho_{6S}$) exhibited large biases, with the TOA and DT methods underestimating surface reflectance and the 6S method overestimating surface reflectance (Table 3). These biases result in $RMSE_\rho$ of between 2.7% – 7.0% reflectance (here and hereafter all reflectance errors will be reported in terms of absolute percent reflectance units). Correction of

the apparent surface reflection using known reflectance reduces the bias to less than 0.06% and reduces the $RMSE_{\rho}$ to 0.32% - 4.0%. In general, the 6S method produced the smallest overall $RMSE_{\rho}$, though correction brought error using all methods into near parity. Uncorrected error showed little dependence on instrument, though corrected OLI did result in the lowest error for both the corrected and uncorrected cases.

For all instruments and all surface reflectance retrieval methods, solar zenith angle was positively correlated with $RMSE_{\rho}$ meaning solar zenith angles closer to nadir resulted in lower $RMSE_{\rho}$ (Table 3). For the TOA and DT methods, visibility was negatively correlated with $RMSE_{\rho}$ meaning lower visibility conditions led to greater spectral error. The 6S method was impervious to visibility, but did show sensitivity, at least for TM and ETM+, to water vapor. Although correction generally preserves the correlations between visibility and solar zenith angle, the absolute value of the slopes of the relationships were greatly reduced meaning that the dependence upon error was much smaller (though in some cases still significant) than in the uncorrected case.

The correction using known reflectance, which reduced $RMSE_{\rho}$ for all reflectance retrieval methods (Table 3), appears to augment the impact of improved SNR and corrected OLI reflectance produces the best retrievals with errors < 1% for all reflectance retrieval methods. The impact of reflectance retrieval method is best seen for the low-noise OLI instrument, with 6S producing the best uncorrected reflectance averaged over all bands (Table 3). The advantage of the more sophisticated 6S method disappears, however, with correction using known reflection. This probably results from the fact that the DT method accounts for atmospheric effects directly, whereas the 6S approach relies on estimates of transmittance and reflection due to scattering. Since the approach used here uses known atmospheric parameters, which are calculated directly

from MODIS and also used for the calculation of ρ_{TOA} , and not estimated from ancillary sources as in the operational cases (i.e., for MODIS and Landsat), our results probably underestimate the amount of error in the 6S retrievals. However, they do set a lower bound on error due to the propagation of instrument noise through the 6S equations, and in this way contributes to understanding the error budget of the operational Landsat and MODIS reflectance retrieval approaches.

The TOA method produced high $RMSE_{\rho}$ in the red, NIR, and SWIR for all instruments, though the error was generally lowest for OLI (Table 4). TOA spectral bias, ME_{ρ} , was highest, in an absolute sense, for shorter wavelengths and decreased with wavelength. This is the result of impact of atmospheric scattering that is strongest in the blue and decreases with increasing wavelength. Using the DT method, all instruments produced very similar $RMSE_{\rho}$ and ME_{ρ} . All bands for all instruments displayed negative biases (predicted reflectance less than actual reflectance). The responses of the instruments differed in the NIR and SWIR. In particular, OLI and MODIS produced smaller error and smaller negative biases. This was particularly marked in the SWIR2, where the reflectance of NPV and soil differ the most (Figure 2). The 6S method produced the highest errors, as well as the largest biases, in the SWIR. These were offset by low errors and moderate biases of opposite sign in the shorter wavelengths, resulting in the net lowest $RMSE_{\rho}$ (Table 3).

In Case 1, GV showed the lowest $RMSE_f$ and smallest bias (lowest absolute value of ME_f) compared to NPV and soil, which exhibited near-equal $RMSE_f$ (Table 5). $RMSE_f$ and ME_f for GV did not depend strongly on reflectance retrieval method or instrument, with the exception of OLI and MODIS in the uncorrected 6S case, which exhibit the GV $RMSE_f$ double that of the TOA and DT methods. The uncorrected TOA method resulted in extremely high errors for NPV

and soil with NPV exhibiting positive bias and soil exhibiting a slightly stronger (more negative) bias. The net negative bias (i.e. the sum of ME_f for all cover types) for the TOA and DT methods mimics the negative ME_p for these methods because lower total reflectance must result in lower fractions. Correction of the apparent surface reflectance significantly reduced the $RMSE_f$ and nearly eliminated bias, except for the TOA method, where considerable error in NPV and soil fractions remained. For both uncorrected and corrected reflectance, the DT method resulted in lower errors than the 6S method.

The variability in unmixed fractional cover was strongly dependent upon instrument with average standard deviation decreasing with instrument noise (Table 6). The results shown are for the uncorrected reflectance case, but because the correction method did not reduce the impact of noise, results for the uncorrected reflectance are similar. For any instrument, NPV and soil fractions exhibited the highest (and nearly equal) average standard deviation. For a particular instrument, the DT method generally produced the least variable NPV and soil fraction estimates and the 6S method produced the highest.

A clear result of the research is that the superior noise characteristics of Landsat 8 OLI over its Landsat 5 and 7 predecessors translates directly into better stability of surface fractional cover retrievals, all other things being equal (Table 6). The additional NIR band in MODIS did not significantly change the fractional cover retrievals, except where it may have reduced $RMSE_f$ slightly in the different unmixing cases (Table 7). In both unmixing cases and for all ground cover types, MODIS $RMSE_f$ and the magnitude of ME_f was less than or equal to the $RMSE_f$ and ME_f of the other instruments.

We investigated the impact of unmixing approach (i.e. simple SMA [Case 2] vs. MESMA [Case 3]) on fractional cover error, and how these errors were augmented by (uncorrected)

reflectance retrieval and (uncorrected) reflectance retrieval of noisy L_{TOA} spectra (Table 7). Consistent with Case 1, unmixing of retrieved reflectance (Table 5), the DT reflectance retrieval method produced the lowest errors, and only results from the DT method are shown in Table 7. In all cases, $RMSE_f$ was lowest for GV, compared to NPV and soil. This is consistent with our Case 1 results. $RMSE_f$ was nearly the same for both NPV and soil and displayed, along with GV, no dependence upon instrument. For the MESMA unmixing case (Case 3), the biases of NPV and soil were nearly equal but opposite.

When unmixing the original ground spectra, ρ_{actual} , the simple SMA unmixing case (Case 2) produced slightly higher NPV and soil $RMSE_f$ than the MESMA unmixing case (Case 3) but resulted in no bias for any cover type (Table 7). When reflectance retrieval was added (i.e., unmixing of $\rho_{TOA,DT}$ retrieved from L_{TOA}), $RMSE_f$ increased for NPV and GV for all instruments, but $RMSE_f$ actually went down for soil for all instruments except OLI, which had produced the highest $RMSE_f$ for soil when unmixing ρ_{actual} . Again, Case 2 unmixing resulted in higher $RMSE_f$ than Case 3, but produced biases that were particularly large for NPV. When noise was added (i.e., unmixing of $\rho_{TOA,DT}$ retrieved from $L_{TOA,noisy}$), $RMSE_f$ increased for all cover types for TM and ETM+. Due to the low noise of these instruments, $RMSE_f$ in the presence of noise for OLI and MODIS remained nearly identical to those produced by unmixing of $\rho_{TOA,DT}$ retrieved from L_{TOA} .

There were few clear, consistent relationships between $RMSE_f$ for Case 3 and solar zenith angle, visibility, water vapor content (Table 8). However, generally solar zenith and visibility exerted a stronger influence upon $RMSE_f$ than water vapor content, though this is less true for the 6S method. Results showed no clear dependence upon instrument and coefficients showed no relationship to those calculated for $RMSE_\rho$ (Table 3). For the TOA reflectance retrieval method,

solar zenith angle was generally positive, the only exception being TM estimation of GV fractional cover, but in this case, the negative coefficient is two orders of magnitude smaller than the positive coefficients found for NPV and soil. For estimates of NPV and soil fractional cover, the highest coefficients were observed for solar zenith angle. The DT and 6S methods significantly reduced (i.e., decreased the magnitude of the multiple regression coefficient) or eliminated this dependence of NPV and soil $RMSE_f$ on solar zenith angle, but they increased the coefficients for some of the instruments.

The effect of atmospheric conditions upon fractional cover retrieval varied by instrument, reflectance retrieval method, and ground component, but in nearly all cases, there was a significant relationship between $RMSE_f$ and atmospheric conditions (Table 8). The average over all instruments of multiple- R^2 for the regression of $RMSE_f$ against normalized atmospheric factors (solar zenith angle, visibility, and water vapor content) is a rough index of which atmospheric correction method was most effective at removing the influence of the atmosphere. This average for the TOA method was highest (0.82). For DT and 6S the average was 0.60 and 0.69, respectively, consistent with our finding that the lowest fractional cover errors were associated with the DT method and the highest errors were associated with the TOA method. For the TOA method, there was a significant relationship with at least two of the atmospheric factors. The fact that this method does not attempt to remove atmospheric factors, resulting in atmosphere-dependent apparent reflectance, was clearly propagated through the spectral mixing to yield high errors.

The lack of consistent patterns among the coefficients of multiple regression of $RMSE_f$ against normalized atmospheric factors is partially due to the fact that instrument noise, since it is random, will tend to decrease the strength of the correlations. Thus, it is best to concentrate on

results primarily for OLI, due to its low noise, and MODIS, due to its additional spectral band in the NIR as well as its low noise. Because the DT method produces fractional cover with the lowest $RMSE_f$, we will also focus only on these results (Table 8). In this context, NPV error appears to exhibit the strongest dependence upon atmospheric factors (with $R^2 = 0.74$ and $R^2 = 0.82$, for OLI and MODIS, respectively), though the impact of solar zenith angle and visibility are equally, but oppositely, weighted. The error arising from solar zenith angle is not simply a consequence of the illumination of the surface, since this effect is eliminated in Equations (4) and (5) and would create negative biases for all ground cover components, which we do not see. Instead, the opposite coefficients for solar zenith angle and visibility arise from fact that a high solar zenith angle increases atmospheric path length, whereas high visibility translates to low atmospheric scattering. It should be noted that the ground surface is assumed to be flat and horizontal, meaning that there are no shadows cast by vertical objects and no slope effect. Because shadowing depends on solar zenith angle, a more complicated approach involving vertical objects would likely see additional effects due to shadowing. Error in the other two ground components (GV and soil) is slightly more dependent upon visibility, but none of the error of the ground components is significantly related to water vapor. This is not surprising, because multispectral bands are largely chosen to avoid water vapor bands.

An error budget can be produced that accounts for the errors arising from unmixing approach, atmospheric retrieval, and instrument noise (Table 9). Class 1 error is due solely to unmixing method. Class 2 error is due to reflectance retrieval. Class 3 is error that arises from instrument noise.

MESMA unmixing (Case 3) of NPV and soil improved fractional cover estimates of these ground components (reduced class 1 error), while slightly degrading the estimate of GV

fractional cover (increased class 1 error). This effect was not strikingly instrument-dependent, though the presence of an additional NIR band in MODIS did reduce difference in this instrument compared to others. It would be easy to over-interpret this result, but it remains to be seen whether and to what extent this effect is dependent upon endmember selection.

Addition of atmospheric retrieval (DT method) mostly added class 2 error to fractional cover estimates for Case 2 (Table 9). For MESMA (Case 3), the additional class 2 was small (absolute values ± 0.03), with slight reductions in class 2 error (i.e., negative values) due to the interaction of endmember selection with instrument bands. We do not consider these additions or reductions in error to be large enough to warrant scrutiny without a more thorough investigation of endmember selection. However, Case 2 (simple unmixing employing the average of ground spectra used to produce ρ_{TOA}), the DT atmospheric method mostly adds class 2 error for GV and NPV. Surprisingly, reflectance retrieval led to no change or slight improvement (for TM and ETM+) in the estimation of soil fraction. This result implies that soil fractional cover estimation is largely impervious to reflectance retrieval.

This cannot simply be because atmospheric correction does not impact the ability to distinguish spectrally between NPV and soil; the class 2 error in SMA (Case 2) NPV fractional cover increases. The increase in class 2 error for Case 2 NPV fractional cover estimates is associated with a large underestimate (i.e., negative ME_f) in NPV fractional cover estimates (Table 7). So, DT atmospheric retrieval results in underestimates of NPV fractional cover while simultaneously barely affecting the estimates of GV and soil. This effect is particularly prominent for OLI and MODIS. Since the constraint that fractional cover for all cover types must sum to one (Equation 10) was *not* enforced in this study, the underestimation in NPV does not necessarily lead to an overestimation of the other fractional cover types. The fact that the error

and bias are seen most prominently in a single ground cover fraction (NPV) indicates that they arise from differences in a few bands, rather than systematically across the entire spectrum, and indeed no systematic difference is seen across the entire spectrum (Table 3).

When individual bands are considered, however, an explanation for the high NPV error and bias for OLI and MODIS emerges (Table 4). OLI and, to a lesser extent, MODIS exhibit a smaller bias in the NIR and SWIR bands. As a result, retrieved reflectance spectra from this instrument will have a slightly different shape that, when used for unmixing, clearly results in underestimation for these instruments. The signs of the various biases support this: by producing higher reflectance in the SWIR2 (i.e., smaller negative biases), the resulting spectrum looks less like NPV, which is differentiated from soil in this region by having lower reflectance than soil.

These large class 2 errors in NPV fractional cover for OLI and MODIS are only present in Case 2. They do not arise in when MESMA is used (Case 3). We speculate that this is because allowing variability in the endmembers reduces the impact of deformations in the retrieved spectrum because the MESMA endmembers themselves have slightly different shapes.

The dominant error for the earlier instruments (TM and ETM+) is instrument noise and the class 3 error that arises from instrument noise is explainable readily from the SNR of the instruments themselves (Table 2), with error decreasing with instrument SNR (Table 9). In fact, the level of noise for OLI and MODIS does not contribute any error to spectral unmixing estimates of fractional cover.

Discussion

The aim of this study was to explore how the spectral and noise characteristics of spaceborne multispectral remote sensing instruments interact with geometric and atmospheric conditions when the data is used for spectral unmixing of apparent surface reflectance.

It is not surprising that the TOA reflectance retrieval method produces the largest (uncorrected) $RMSE_{\rho}$ across the entire spectrum (Table 3) because this approach fails to take into account atmospheric conditions. The more-or-less constant negative biases (within a few reflectance units) across the spectrum for all instruments with the DT method indicate that this method is able to remove the effect of path radiance on reflectance retrieval. These constant negative biases also result in retrieved slightly darkened reflectance spectra that have nearly the same shape as the original surface reflectance.

Although it produced the lowest average spectral error for most instruments, the state-of-the-art surface reflectance retrieval method based on the 6S radiative transfer code (e.g., Masek et al. 2008), which is used operationally to produce reflectance for MODIS and Landsat, produced higher fractional cover error than the DT subtraction method, with or without correction for known reflectance, though correction makes the difference between the two negligible (Table 5). This is consistent with the findings of Song et al. (2001) who found that more complicated algorithms do not necessarily lead to improved performance of classification and change detection. Also, the 6S method appears to exacerbate instrument noise leading to greater variability in unmixed fractions than the DT method (Table 6). This may be partly due to the treatment of water vapor in the 6S method. Though 6S does well in reducing spectral error due to visibility, it alone among methods produced spectral error, $RMSE_{\rho}$ that was significantly related to atmospheric water vapor content.

The higher NPV and soil fractional cover error from the 6S method compared to the DT method is intriguing in light of the fact that the 6S reflectance inversion method actually produces lower spectral error over all bands than the DT method. This appears to be a result of the fact the different bias for individual bands produced by the methods (Table 4). Whereas the

DT biases are uniformly negative, the 6S biases shift from positive in the visible to strongly negative in the SWIR. Thus, although the DT reflectance retrievals are biased, they are consistently so, resulting in a reflectance spectrum that are slightly darkened but closely resemble the original. In contrast, the varying biases for the 6S method results in a spectral shape that resembles less the original ground reflectance (ρ_{actual}) and thus results in higher fractional cover error. Our results suggest that either DT correction or correction of 6S-derived surface reflectances based on known reflectance are optimal for SMA.

The 6S approach is used for reflectance retrieval in publically available and widely used MODIS (including the MOD09/MYD09, surface reflectance with atmospheric correction, or MCD43, nadir BRDF-adjusted reflectance, products) and Landsat products (including the Landsat surface reflectance products available at: http://landsat.usgs.gov/CDR_LSR.php). Our results suggest that care must be taken in the use of SMA of GV, NPV, and soil of these reflectance products. Where possible, the 6S-derived reflectance should be further corrected using the reflectance of a known *in situ* target. This is especially feasible with Landsat, with its smaller IFOV compared to MODIS. Additional DT correction of 6S reflectance may also improve fractional cover estimates because it has the capacity to counteract systematic error in the image; however, this was not explicitly tested in this study.

ρ_{TOA} should not be used for spectral unmixing to produce absolute vegetation fractions, especially when correction based on known ground reflectance is unavailable; it resulted in very high fractional cover errors, particularly for NPV and soil and even with correction (Table 5). This limitation may be somewhat relaxed when image endmembers (i.e. pixel spectra taken from the image itself where the pixels are assumed to be covered entirely by one cover type) are used,

because the image endmembers will have the same systematic errors as the rest of the scene, particularly at shorter wavelengths where atmospheric scattering creates the greatest error.

Our results present a strong argument for the development of multispectral instruments with additional bands and deployment of spaceborne imaging spectrometers, such as the planned HypsIRI. In MODIS, the addition of a second NIR band reduces the unmixing error because the per-band importance of any spectral difference is decreased as the number of bands increases. The overdetermined nature of spectral unmixing with a large number of bands also will likely result in better retrievals of fractional cover because the instrument noise for each band can be offset by others, at least in an average sense.

Smith et al. (1990) found that the coefficient of determination (R^2) between vegetation fraction from SMA and vegetation from the field was 0.80 - 0.91 using Landsat 5 TM. With instrument noise, the R^2 for Case 2 (uncorrected, DT) GV unmixing is 0.52, 0.78, and 0.91 for Landsat 5, 7, and 8, respectively. Thus, in comparison with the results of Smith et al. (1990) for Landsat 5, we find greater variability (lower R^2) due to instrument noise, suggesting that the effective noise level from Smith et al. (1990) is lower than that used here for Landsat 5 TM. Indeed, to the extent that the comparison between Case 2 unmixing is appropriate, the effective level of noise for Landsat 5 might be closer to that of Landsat 7 ETM+ or Landsat 8 OLI. Likewise, Elmore et al. (2000) found, for sites in the Owens Valley, California, that GV could be estimated with Landsat 5 TM at a level of 4% absolute cover. This is consistent with our findings that GV fractions derived from $\rho_{TOA,DT}$ from L_{TOA} can be estimated at about 4-5% absolute (Table 7), though, our estimate of noise for Landsat 5 TM suggests that error can be much higher. The discrepancy between the results of Elmore et al. (2000) and GV fractions derived from $\rho_{TOA,DT}$ from $L_{TOA,noisy}$ further suggests that the effective noise for their study was much lower than that

estimated by Helder et al. (2004) and used here. The relatively low effective Landsat 5 TM error suggested by these studies compared to errors estimated from other sources (e.g., Landsat Data Continuity Mission for Landsat 7 and Helder et al. 2004) suggests that the SNRs used here (Table 2) might be too low, and that the Landsat 7 or 8 SNRs might be better representations of the effective SNR for Landsat 5 for the purpose of unmixing. Indeed, the values of SNR used for Landsat 5 in Sabol et al. (1992) are higher (e.g., 80-100 in the VNIR) than those predicted from Helder et al. (2004). Although the source of the SNR in Sabol et al. (1992) is unattributed, our results suggest that their values of SNR might be more realistic for Landsat 5 than those used here. The noise values for Landsat 5 used here, therefore, should be considered worst-case values, with actual noise levels potentially being higher for real Landsat 5 data.

Okin et al. (2013) report minimum fractional cover errors using SMA for unmixing MODIS normalized BRDF-adjusted reflectance (NBAR) data from agricultural fields in southern Australia of 0.08 (0.0), 0.17 (-0.14), and 0.19 (0.14) for GV, NPV, and soil, respectively (numbers in parentheses represent ME_f). MESMA produced minimum fractional cover errors of 0.07 (-0.02), 0.12 (-0.04), and 0.13 (0.06) for GV, NPV, and soil, respectively. Likewise, for unmixing of MODIS NBAR data from structurally complex southern African savannas, Meyer et al.'s (2015) SMA analysis produced $RMSE_f$ (ME_f) of 0.10 (0.0), 0.29 (0.25), and 0.29 (-0.25) for GV, NPV, and soil, respectively. Their MESMA analysis produced $RMSE_f$ (ME_f) of 0.09 (0.0), 0.16 (0.08), and 0.17 (-0.08) for GV, NPV, and soil, respectively. In contrast, here we estimate that MODIS SMA (Case 2) produces $RMSE_f$ (ME_f) of 0.04 (-0.02), 0.26 (-0.21), and 0.17 (0.10) for GV, NPV, and soil, respectively, and that MESMA (Case 3) produces $RMSE_f$ (ME_f) of 0.07 (-0.05), 0.19 (-0.11), and 0.16 (0.05) for GV, NPV, and soil, respectively.

Okin et al. (2013), Meyer et al. (2015) and the present study agree that lower errors should result from estimates of GV fractional cover compared to NPV and soil. They also agree that the biases in estimates of NPV and soil fractional cover are of opposite sign. These results are all consistent with the analysis of Sabol et al. (1992) who highlighted the importance of spectral contrast (i.e., the difference between endmembers) in unmixing. They conclude that that low contrast (i.e., more similar spectra, such as with NPV and soil) decreases the detectability of low-abundance endmembers and increases overall error. Our results are closer to those of Okin et al. (2013), which have lower error than those from savannas, possibly due to the structural complexity of the latter.

That the MESMA results from Okin et al. (2013) improve slightly upon the SMA results from that study, highlights the importance of providing for spectral variation in analytical procedures that use the spectral signature to retrieve fractional cover (Song 2005; Somers et al. 2011). Our study augments this conclusion, as our MESMA fractional cover estimates resulted in lower error than the SMA estimates, even in the presence of high instrumental noise. This was true even though the endmember for the SMA were derived directly from those used to produce TOA radiance (as an average). We hypothesize that allowing variation in endmembers can counteract subtle effects of instrument noise and error due to reflectance retrieval. Since this was not an exhaustive study of the effect of endmember selection, it will take further work to investigate this hypothesis, but our results do suggest that in the absence of correction to known reflectance, that fractional cover error of ~ 0.06 for GV should be expected as a minimum (i.e., the minimum value in the final column of Table 7 GV), whereas NPV and soil might only be retrievable within any mixed pixel of Landsat or MODIS scale with errors > 0.16 (i.e., the minimum value in the last column in Table 7 for NPV and soil). The fractional cover error due to

unmixing of corrected reflectance (GV ~ 0.01 and NPV and soil ~ 0.03 , Table 6 minimum values for each endmember) might represent an absolute minimum for fractional cover error at this scale.

Our results confirm those of Huete and Jackson (1988), who found that decreasing visibility led to a reduction in the ratio vegetation index (i.e., the ratio of radiance in the TM red channel to the radiance in the TM NIR channel which will covary positively with NDVI). In other words, Huete and Jackson (1988) found that radiance-derived vegetation indices, without atmospheric correction, will decrease the apparent GV cover, as measured by a vegetation index. Our results (Table 8) indicate a positive slope between visibility and derived GV cover in the TOA case, and are therefore consistent with the findings of Huete and Jackson (1988). Huete and Jackson (1988) also showed that this effect is stronger at higher SZAs, consistent with the negative relationship between GV cover and SZA found in this study (Table 8). NPV error appears to exhibit the strongest dependence upon atmospheric factors. Since fractional cover errors are generally high for this ground cover component, and since NPV is often confused with soil, atmospheric conditions must be taken into account when assessing the error of NPV (and soil) fractions. This is especially true in desert areas where dust can decrease visibility, near urban areas with atmospheric pollution, and in other regions where atmospheric aerosols increase the turbidity of the atmosphere, especially during times of year or locations with high SZA.

Conclusion

The purpose of this study was to examine the impact of instrument, instrument noise, atmospheric conditions, and reflectance retrieval method on estimation of fractional cover of GV, NPV, and soil. To some extent, all of these factors can lead to error in fractional cover estimates. But, it is clear from our results that instrument noise has a direct impact on the

accuracy of surface reflectance retrieval and fractional cover estimation. There is also some suggestion from our results that the additional band in MODIS significantly improves fractional cover estimation due in part, we think, to the dilution of noise effects provided by the additional band. This result argues strongly, though perhaps not surprisingly, for development of instruments with additional spectral bands; the current SNR of OLI is clearly sufficient to not contribute to fractional cover error, all other things being equal.

Contrary to our expectations, better overall retrieval of surface reflectance does not necessarily lead to improved fractional cover estimation. Biases that enter surface reflectance at the band level leads to distortions of the spectral shape that can lead to errors in fractional cover estimates. We find that, for fractional cover estimates, it is better to have higher overall spectral error if the biases are equal across bands than to have a lower overall spectral error with varying per-band biases. In our study, this appears to affect NPV the most, but in practice, we speculate that soil fractional cover estimates may also be vulnerable to this effect, particularly if constraints are placed upon the sum of fractions. The spectra of NPV and soil are similar enough that small distortions in spectral shape could result in errors in fractional cover estimates of either one, or both.

Distortions in spectral shape due to reflectance retrieval methods appear to be partially offset by allowing variability in endmembers, as we did through the use of MESMA. Even in cases where the MESMA endmembers were not directly related to those used in the simulation of TOA radiance, the use of multiple endmembers for each ground component appeared to dilute many of the sources of error that we observed, including instrument noise. The endmembers we used in our Case 3 MESMA were from the same field sites as those used for estimation of TOA radiance and were thus closely related to the original spectra. If this is the reason that MESMA

reduced fractional cover error, then this fact argues strongly for collection of *in situ* spectra when possible. However, we cannot say with certainty that this improvement would not also be seen with endmember spectra that were less closely related. We hypothesize, indeed, that it is the variation itself, not necessarily how close the endmembers are to the actual ground spectra, that improves fractional cover estimates in the presence of other sources of error, such as instrument noise and reflectance retrieval. More study into endmember choice is required to evaluate this hypothesis, perhaps using a simulation study like this one, but with fewer atmospheric conditions and reflectance retrieval approaches. Okin et al. (2001) did study this phenomenon to some degree and discovered, in particular, the possibility of “coupling” between certain spectra such that a combination of two endmember spectra can look like a combination of actual ground spectra. This leads to systematic error in fractional cover estimates, and any study of endmember choice must evaluate the impact of spectral coupling while also providing ways to obviate its effects.

Based on our results, a set of recommendations may be made for optimal multispectral unmixing of GV, NPV, and soil:

- 1) Atmospheric retrieval method matters. DT is optimal, especially when corrected. When DT is not possible, as when imagery has already been corrected before distribution, then correction of reflectance through calibration to a known *in situ* spectrum will improve fractional cover retrievals. Additional DT correction of 6S-derived reflectance also has the potential to improve reflectance retrieval, though this was not explicitly evaluated in this study.

- 2) Reflectance correction will improve results. Since correction to a known reflectance, usually of a pseudo-invariant ground target, accounts for systematic per-band errors due to

atmospheric conditions, especially for instruments with high SNR, we suggest the implementation of this procedure prior to spectral unmixing in all cases in which it is possible.

3) SZA influences the impact of atmospheric conditions on reflectance retrieval and fractional over estimates. Therefore, care must be taken when comparing fractions retrieved at different times of the year or at different latitudes.

4) Visibility matters. If possible, avoidance of times and locations with high atmospheric turbidity is advised.

5) Inclusion of spectral variability can counteract reflectance error. Whenever possible, methods that include spectral variability, such as MESMA, should be used to counteract the impact of instrument noise and suboptimal reflectance retrieval.

There are many sources of error that we did not include in this study including the potential of noise to actually increase error during reflectance correction and the need to estimate atmospheric parameters in the 6S method. These errors are likely to be additive on top of the errors investigated here. As a result, the error bounds determined here (uncorrected: ~0.06 for GV ~0.16 for NPV and soil; uncorrected ~0.01 for GV and ~0.03 for NPV and soil ~0.03) should be considered conservative estimates of minimum error.

In truth, an error of ~0.16 for fractional cover might be too high for many applications. Asner and Lobell (2000) found lower error using imaging spectroscopy data in the SWIR2 and they suggest that more multispectral bands in the SWIR2 might significantly improve fractional cover estimates of NPV and soil. Although we did not investigate directly the impact of more SWIR2 bands, the addition of these bands in new generations of multispectral sensors, until they can be replaced by spaceborne imaging spectrometers with high SNR, would likely help distinguish between soil and NPV to reduce the error associated with estimates of both. But, our results warn

that, without equal-bias, low-error reflectance retrieval, additional bands may not significantly contribute to improved fractional cover estimates.

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Figure Captions

Figure 1. Schematic of experimental approach. First at-sensor TOA radiance was simulated for a variety of atmospheric and geometric conditions, and instrument noise was added to the simulated signal. Then, reflectance was estimated, and this was used to estimate fractional cover of GV, NPV, and soil. Estimated fractions were compared against fractions used to simulate TOA radiance.

Figure 2. Spectra of GV (green), NPV (orange), and soil (brown) used to create TOA radiance (solid) and average of these spectra (dashed lines) used in Case 2 for unmixing.

Figure 3. Endmember spectra of GV (green), NPV (orange), and soil (brown) used for unmixing in Case 3.

Table 1: Variable MODTRAN parameters used to produce model atmospheres.

Julian Day	(Date)	z	w in g cm^{-2}	v in km
79	(March 20)	42.2°	0.5	10
171	(June 20)	22.9°	1.0	20
355	(December 21)	62.0°	2.0	50

Meteorological range = $1.3 * \text{observed visibility } (v)$.

Table 2: Instrument signal-to-noise ratios (SNRs) used in this study

Band	Landsat 5 TM	Landsat 7 ETM+	Landsat 8 OLI	MODIS
Blue	32	39	355	243
Green	17	37	296	228
Red	18	26	222	128
NIR1 (800 nm)	15	34	199	201
NIR2 (1200 nm)	-	-	-	74
SWIR1	26	36	261	275
SWIR2	18	27	326	110

Table 3: Spectral error ($RMSE_{\rho}$, ME_{ρ} ; Reflectance Units x 100) for different instruments and different reflectance retrieval methods, and coefficients of regression of $RMSE_{\rho}$ against normalized water vapor, normalized visibility and normalized solar zenith angle. All combinations of z , w , and v are included in the calculations. Only regression coefficients significant at the 95% level are reported.

		Not corrected using known reflectance			Corrected using known reflectance		
		TOA	DT	6S	TOA	DT	6S
Landsat 5 TM	All Bands ($RMSE_{\rho}$, ME_{ρ})	6.19,-2.20	6.99,-5.91	6.56,4.12	3.74,-0.05	4.01,-0.05	3.85,-0.05
	Norm. WV ^a (slope, intercept)			-1.58,7.26			
	Norm. Vis. ^a (slope, intercept)	-1.13,6.66	-2.00,7.82		-0.05,3.77	-0.28,4.13	-0.10,3.89
	Norm. SZA ^a (slope, intercept)	1.49,5.45	2.09,5.96	1.49,5.83	0.05,3.72	0.24,3.89	0.12,3.79
Landsat 7 ETM+	All Bands ($RMSE_{\rho}$, ME_{ρ})	5.47,-1.72	6.14,-5.58	4.53,3.20	2.35,-0.05	2.41,-0.05	2.32,-0.05
	Norm. WV ^a (slope, intercept)			-1.20,5.07			
	Norm. Vis. ^a (slope, intercept)	-1.28,6.00	-2.14,7.04		-0.09,2.38	-0.16,2.47	-0.07,2.35
	Norm. SZA ^a (slope, intercept)	1.70,4.63	2.24,5.04	1.46,3.81	0.09,2.30	0.14,2.33	0.08,2.28
Landsat 8 OLI	All Bands ($RMSE_{\rho}$, ME_{ρ})	4.21,-1.00	4.92,-4.79	2.69,1.69	0.85,-0.05	0.32,-0.05	0.36,-0.05
	Norm. WV ^a (slope, intercept)						
	Norm. Vis. ^a (slope, intercept)	-1.38,4.78	-2.30,5.88		-0.24,0.95	-0.03,0.33	-0.12,0.41
	Norm. SZA ^a (slope, intercept)	1.64,3.40	2.21,3.83	1.27,2.06	0.24,0.73		0.11,0.30
MODIS	All Bands ($RMSE_{\rho}$, ME_{ρ})	4.65,-1.08	4.93,-4.67	3.55,1.91	1.40,-0.06	0.94,-0.05	0.96,-0.06
	Norm. WV ^a (slope, intercept)						
	Norm. Vis. ^a (slope, intercept)	-1.92,5.45	-2.67,6.04				
	Norm. SZA ^a (slope, intercept)	1.73,3.80	2.19,3.85	1.44,2.84			

^a Normalization of independent variable X done using: $X(\text{norm}) = (X - \min(x)) / (\max(x) - \min(x))$

Table 4: Average spectral error ($RMSE_{\rho}$, ME_{ρ} ; Reflectance Units x 100) for each band of the instruments considered. Only results for uncorrected reflectance are shown. All combinations of z , w , and v are included in the averages.

		Blue	Green	RED	NIR1	NIR2	SWIR1	SWIR2
TOA	Landsat 5 TM	6.75 (6.60)	2.48 (0.33)	3.60 (-2.03)	6.95 (-5.08)	-	7.67 (-6.89)	7.55 (-6.15)
	Landsat 7 ETM+	7.28 (7.17)	1.61 (0.94)	2.87 (-1.87)	5.11 (-4.61)	-	5.55 (-4.93)	7.62 (-7.00)
	Landsat 8 OLI	6.92 (6.87)	1.16 (0.88)	1.74 (-1.49)	2.95 (-2.91)	-	4.64 (-4.60)	4.79 (-4.73)
	MODIS	8.30 (8.25)	1.77 (1.61)	2.01 (-1.75)	3.15 (-3.11)	4.62 (-4.45)	3.32 (-3.29)	4.65 (-4.52)
DT	Landsat 5 TM	3.57 (-3.29)	5.96 (-5.42)	6.66 (-5.92)	8.65 (-7.19)	-	8.05 (-7.30)	7.72 (-6.36)
	Landsat 7 ETM+	3.47 (-3.23)	5.29 (-5.13)	6.17 (-5.76)	7.11 (-6.76)	-	5.95 (-5.37)	7.81 (-7.21)
	Landsat 8 OLI	3.35 (-3.24)	5.17 (-5.12)	5.56 (-5.49)	4.91 (-4.89)	-	5.10 (-5.07)	5.01 (-4.95)
	MODIS	3.18 (-3.05)	4.73 (-4.68)	5.93 (-5.84)	5.16 (-5.14)	5.42 (-5.28)	3.78 (-3.75)	4.88 (-4.76)
6S	Landsat 5 TM	2.40 (1.63)	3.86 (1.96)	3.99 (1.63)	8.48 (5.73)	-	8.35 (7.10)	8.83 (6.67)
	Landsat 7 ETM+	2.25 (1.66)	2.52 (1.99)	3.08 (1.73)	5.32 (4.57)	-	4.17 (2.97)	7.40 (6.29)
	Landsat 8 OLI	1.59 (1.56)	1.84 (1.82)	1.85 (1.81)	0.57 (-0.27)	-	0.57 (-0.37)	5.61 (5.55)
	MODIS	2.05 (2.02)	3.16 (3.14)	3.32 (3.26)	1.13 (1.03)	1.46 (-0.64)	1.41 (1.36)	9.81 (9.64)

Table 5: Average fractional cover error due to surface reflectance inversion (Case 1). All combinations of z , w , and v are included in the averages.

Cover Type	Instrument	RMSE _f (ME _f) Due to Surface Reflectance Inversion Method (Uncorrected)			RMSE _f (ME _f) Due to Surface Reflectance Inversion Method (Corrected)		
		TOA	DT	6S	TOA	DT	6S
GV	Landsat 5 TM	0.04 (0.01)	0.05 (-0.03)	0.06 (0.06)	0.01 (0.00)	0.00 (0.00)	0.00 (0.00)
	Landsat 7 ETM+	0.04 (0.01)	0.04 (-0.03)	0.05 (0.04)	0.01 (0.00)	0.00 (0.00)	0.00 (0.00)
	Landsat 8 OLI	0.04 (0.03)	0.03 (0.00)	0.08 (-0.08)	0.01 (0.00)	0.00 (0.00)	0.00 (0.00)
	MODIS	0.04 (0.03)	0.04 (-0.02)	0.08 (-0.07)	0.01 (0.00)	0.00 (0.00)	0.00 (0.00)
NPV	Landsat 5 TM	0.76 (0.72)	0.15 (-0.08)	0.26 (0.13)	0.12 (0.01)	0.01 (0.00)	0.03 (0.00)
	Landsat 7 ETM+	0.57 (0.54)	0.18 (-0.04)	0.29 (0.06)	0.13 (0.01)	0.01 (0.00)	0.03 (0.00)
	Landsat 8 OLI	0.63 (0.60)	0.18 (-0.10)	0.33 (0.08)	0.13 (0.00)	0.01 (0.00)	0.03 (0.00)
	MODIS	0.76 (0.72)	0.17 (-0.07)	0.38 (-0.14)	0.12 (0.01)	0.01 (0.00)	0.03 (0.00)
Soil	Landsat 5 TM	0.89 (-0.85)	0.14 (-0.06)	0.22 (-0.03)	0.12 (-0.02)	0.01 (0.00)	0.03 (0.00)
	Landsat 7 ETM+	0.66 (-0.63)	0.18 (-0.08)	0.26 (0.00)	0.12 (-0.01)	0.01 (0.00)	0.03 (0.00)
	Landsat 8 OLI	0.73 (-0.70)	0.14 (-0.02)	0.29 (-0.01)	0.12 (-0.01)	0.01 (0.00)	0.03 (0.00)
	MODIS	0.85 (-0.81)	0.15 (-0.02)	0.37 (0.20)	0.12 (-0.01)	0.01 (0.00)	0.03 (0.00)

Table 6: Average standard deviation across all endmember/fractional cover combinations (Case 1). All combinations of z, w, and v are included in the averages.

Cover Type	Instrument	Standard Deviation Due to Instrument Noise, uncorrected (corrected)		
		TOA	DT	6S
GV	Landsat 5 TM	0.14 (0.15)	0.14 (0.17)	0.18 (0.16)
	Landsat 7 ETM+	0.07 (0.08)	0.07 (0.08)	0.09 (0.08)
	Landsat 8 OLI	0.01 (0.01)	0.01 (0.01)	0.01 (0.01)
	MODIS	0.02 (0.02)	0.02 (0.02)	0.02 (0.02)
NPV	Landsat 5 TM	0.31 (0.38)	0.29 (0.41)	0.40 (0.40)
	Landsat 7 ETM+	0.23 (0.27)	0.18 (0.29)	0.37 (0.28)
	Landsat 8 OLI	0.07 (0.05)	0.03 (0.03)	0.09 (0.04)
	MODIS	0.08 (0.08)	0.04 (0.06)	0.10 (0.06)
Soil	Landsat 5 TM	0.33 (0.35)	0.27 (0.39)	0.38 (0.37)
	Landsat 7 ETM+	0.25 (0.25)	0.18 (0.28)	0.34 (0.27)
	Landsat 8 OLI	0.08 (0.05)	0.02 (0.03)	0.08 (0.03)
	MODIS	0.09 (0.07)	0.04 (0.06)	0.09 (0.06)

Table 7. Average fractional cover error due to unmixing approach and endmember selection. All combinations of z , w , and v are included in the averages.

Cover Type	Instrument	RMSE _f (ME _f) due solely to unmixing approach (i.e. unmix ρ_{actual})		RMSE _f (ME _f) due to mixture models, with reflectance retrieval (i.e., unmix $\rho_{TOA, DT}$ retrieved from L_{TOA})		RMSE _f (ME _f) due to mixture models, with reflectance retrieval and instrument noise (i.e., unmix $\rho_{TOA, DT}$ retrieved from $L_{TOA, noisy}$)	
		Case 2	Case 3	Case 2	Case 3	Case 2	Case 3
GV	Landsat 5 TM	0.03 (0.00)	0.04 (0.01)	0.05 (-0.03)	0.07 (-0.04)	0.15 (-0.05)	0.15 (-0.05)
	Landsat 7 ETM+	0.02 (0.00)	0.04 (0.01)	0.05 (-0.03)	0.07 (-0.04)	0.08 (-0.03)	0.09 (-0.04)
	Landsat 8 OLI	0.02 (0.00)	0.04 (0.01)	0.04 (-0.01)	0.06 (-0.03)	0.04 (-0.01)	0.06 (-0.03)
	MODIS	0.02 (0.00)	0.04 (0.00)	0.04 (-0.02)	0.07 (-0.05)	0.04 (-0.02)	0.07 (-0.05)
NPV	Landsat 5 TM	0.22 (0.00)	0.17 (0.04)	0.27 (-0.20)	0.18 (-0.09)	0.32 (-0.20)	0.30 (-0.09)
	Landsat 7 ETM+	0.22 (0.00)	0.17 (0.03)	0.25 (-0.18)	0.16 (-0.06)	0.26 (-0.18)	0.23 (-0.05)
	Landsat 8 OLI	0.23 (0.00)	0.17 (0.04)	0.32 (-0.27)	0.19 (-0.12)	0.32 (-0.27)	0.20 (-0.12)
	MODIS	0.19 (0.00)	0.16 (0.01)	0.26 (-0.21)	0.18 (-0.11)	0.26 (-0.21)	0.19 (-0.11)
Soil	Landsat 5 TM	0.21 (0.00)	0.17 (-0.05)	0.18 (0.06)	0.16 (-0.03)	0.26 (0.06)	0.28 (-0.03)
	Landsat 7 ETM+	0.20 (0.00)	0.16 (-0.05)	0.17 (0.04)	0.15 (-0.04)	0.20 (0.04)	0.23 (-0.06)
	Landsat 8 OLI	0.22 (0.00)	0.17 (-0.06)	0.22 (0.14)	0.17 (0.02)	0.22 (0.14)	0.17 (0.02)
	MODIS	0.16 (0.00)	0.14 (-0.02)	0.16 (0.10)	0.16 (0.05)	0.17 (0.10)	0.16 (0.05)

Table 8: Coefficients of multiple regression of $RMSE_f$ against normalized solar zenith angle, normalized visibility, and normalized water vapor. Only coefficients significant at the 95% level are reported. Only fractions from uncorrected reflectance were used for these calculations.

Cover Type	Instrument	TOA					DT					6S				
		norm. SZA ^a	norm. vis. ^a	norm. WV ^a	Const.	R ²	norm. SZA ^a	norm. vis. ^a	norm. WV ^a	Const.	R ²	norm. SZA ^a	norm. vis. ^a	norm. WV ^a	Const.	R ²
GV	Landsat 5 TM	-0.005	0.006	-0.006	0.14	0.91		-0.02		0.15	0.56	0.02		-0.01	0.18	0.85
	Landsat 7 ETM+	0.004	0.003		0.08	0.57	0.02	-0.02		0.09	0.61	0.009		-0.009	0.10	0.86
	Landsat 8 OLI		0.01	0.01	0.04	0.85	0.02	-0.03		0.07	0.61	0.007		-0.02	0.09	0.91
	MODIS	0.007	-0.007		0.05	0.59	0.03	-0.05		0.08	0.75	0.03	-0.02	-0.02	0.11	0.89
NPV	Landsat 5 TM	0.10	-0.07		0.56	0.83			-0.02	0.31	0.44	0.05	-0.04		0.40	0.66
	Landsat 7 ETM+	0.13	-0.06	0.06	0.54	0.90				0.23	0.17	0.03			0.25	0.40
	Landsat 8 OLI	0.09	-0.08		0.40	0.71	0.04	-0.04		0.19	0.74	0.05	-0.04		0.22	0.59
	MODIS	0.11	-0.10		0.38	0.79	0.04	-0.04	-0.02	0.19	0.82	0.04			0.20	0.46
Soil	Landsat 5 TM	0.13	-0.08		0.62	0.86	-0.009	0.01		0.28	0.62	0.03		-0.02	0.38	0.63
	Landsat 7 ETM+	0.15	-0.07	0.08	0.59	0.92		0.01	0.02	0.22	0.81		0.02	-0.02	0.24	0.69
	Landsat 8 OLI	0.11	-0.09		0.44	0.75	0.02	-0.03		0.17	0.69				0.17	0.21
	MODIS	0.13	-0.10		0.38	0.82	0.02	-0.03	-0.02	0.17	0.78		0.04	-0.03	0.17	0.72

^a Normalization of independent variable X done using: $X(\text{norm}) = (X - \min(x)) / (\max(x) - \min(x))$

Table 9. Error budget for GV, NPV, and soil for each instrument (only results from uncorrected unmixing of reflectance retrieved by the DT method are shown)

Cover Type	Instrument	<u>Error class 1:</u> RMSE _f due solely to unmixing approach (i.e., RMSE _f from Case 3 unmixing of ρ_{actual} - RMSE _f from Case 2 unmixing of ρ_{actual})	<u>Error class 2:</u> RMSE _f due to reflectance retrieval (i.e., RMSE _f from unmixing of $\rho_{TOA,DT}$ from L_{TOA} minus RMSE _f from unmixing of ρ_{actual})		<u>Error class 3:</u> RMSE _f due to instrument noise (i.e., RMSE _f from unmixing of unmixing of $\rho_{TOA,DT}$ from $L_{TOA,noisy}$ minus RMSE _f from unmixing of $\rho_{TOA,DT}$ from L_{TOA})		<u>Error class 4:</u> RMSE _f due to reflectance and noise (i.e., RMSE _f from unmixing of unmixing of $\rho_{TOA,DT}$ from $L_{TOA,noisy}$ minus RMSE _f from unmixing of ρ_{actual})	
			Case 2	Case 3	Case 2	Case 3	Case 2	Case 3
GV	Landsat 5 TM	0.02	0.03	0.03	0.09	0.07	0.12	0.10
	Landsat 7 ETM+	0.02	0.03	0.03	0.03	0.03	0.06	0.05
	Landsat 8 OLI	0.02	0.02	0.02	0.00	0.00	0.02	0.02
	MODIS	0.01	0.01	0.03	0.00	0.00	0.02	0.04
NPV	Landsat 5 TM	-0.05	0.04	0.01	0.05	0.12	0.09	0.13
	Landsat 7 ETM+	-0.05	0.03	-0.02	0.02	0.07	0.05	0.06
	Landsat 8 OLI	-0.06	0.09	0.02	0.00	0.00	0.09	0.02
	MODIS	-0.03	0.07	0.02	0.00	0.00	0.07	0.03
Soil	Landsat 5 TM	-0.04	-0.03	0.00	0.08	0.12	0.05	0.12
	Landsat 7 ETM+	-0.04	-0.04	-0.01	0.03	0.08	0.00	0.07
	Landsat 8 OLI	-0.05	0.01	0.00	0.00	0.00	0.01	0.00
	MODIS	-0.02	0.00	0.02	0.00	0.00	0.01	0.02

Figure 1

Figure 2

Figure 3