Nonlinear Spectral Mixture Effects for Photosynthetic/Non-photosynthetic Vegetation Cover Estimates of Typical Desert Vegetation in Western China Version 2

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Abstract

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Protocol

Data and Methods

Step 1.

Study Area

The study area is located the transitional zone (38°37'42.60"N, 102°55'11.25"E) between the oasis and the desert in the western region of Minqin County in the Gansu province along the downstream portion of the Shiyang River. This region consists of temperate continental arid climate zones, and the natural vegetation is mainly desert vegetation. A key characteristic of the desert vegetation is that it contains few species, and only a few layers are present with a simple structure and low productivity. *Nitraria* is short (1–2 m in the mature stage) with an open canopy structure, and it is a type of shrub [20, 21], as shown in **Fig 1**. *Nitraria* shrubs are relatively resistant to sandy and salty conditions and serve as windbreaks across the landscape. These shrubs form a natural ecological barrier in oasis environments in the arid region of western China [22]. *Haloxylon* is tall (1–9 m in the mature stage) with a compact canopy structure, and it is a xeric adapted plant [23, 24] (**Fig 1**). Because of its deep roots, numerous branches, resilience, and adaptability, it is drought resistant and capable of growing in barren soil and areas with invasive sands; hence, it is a very valuable plant resource in arid desert regions. *Haloxylon* is the most common species used in artificial afforestation projects in the western area of the Gansu River basin [25].

Fig 1. **Typical desert vegetation.** (left) *Nitraria* shrubs. (right) *Haloxylon*.

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Spectral Data and Preprocessing

In order to remove the effects of endmember variability, the experimental setup was designed so that endmembers were allowed to vary among plots. For each of the experimental plots, plot-specific bare soil (BS), shadow, PV, and NPV endmembers were defined and used in further analyses. In this research, spectra data for each endmember and canopy mixed spectral were obtained from ground-based field experiments; this involved obtaining specific PV/NPV/BS/shadow endmember spectra in each sample plot so that we could remove the effect of variability among the endmember spectra [11]. Reflectance spectral measurements were acquired on August 25, 2014 (a clear-sky day), within 1 h of local solar noon by using a full-range (350–2500 nm) spectroradiometer with a 25° ASD (Analytic Spectral Devices, Boulder, CO) Spec Pro Field spectrometer. The reflectance was calibrated by using a white spectral panel (Labsphere Inc., North Sutton, NH). During windless, cloudless, and full sunshine conditions, we collected data throughout a stable time period (10:00–14:00) from 20 *Nitraria* plots and 20 *Haloxylon* plots with different ratios of PV to NPV cover, and we measured the canopy spectra and the pure endmembers spectra, as shown in **Fig 2**. We used an orthogonal ruler to determine the center of the plots, and we marked out 1 m diameter circular area to ensure the sample range was consistent. Measurements were taken from nadir at a height of 2.3 m above the earth's surface, which resulted in a field of view (FOV) or a pixel/plot diameter of 1 m from which we obtained the mixed spectral data for the fields, as illustrated in **Fig 2**; meanwhile, we placed the probe above the various typical species endmember surfaces (e.g., *Nitraria*, *Haloxylon*, dry branches, fine sand, shadows) between 0.1 m and 0.02 m so that pure endmember spectra were acquired in each field, as illustrated in **Fig 2**. In this way, each mixed canopy pixel and the specific pure endmember spectra for the field sites were obtained.

Fig 2. Processing of each endmember and mixed canopy spectral data collection in situ. (left) Acquisition of spectral data. (center) Sample selection for Nitraria shrub spectral data. (right) Sample selection for Haloxylon spectral data. PV represents the sunlit and shaded green leaves; NPV represents the sunlit and shaded wood, senescent material, and litter; BS represents the bare soil; shadow represents only the shade on the soil.

Reference Fraction

In this study, photographs were acquired two times by using a digital camera at each field site, in order to avoid out of focus. The photograph with higher quality will be selected, so that the photograph could be used to get the reference fraction accurately. Information on the ground cover composition of each of the measured mixed pixels was extracted from the digital photographs (positioned at nadir) so that the ground cover fraction distribution could be determined. As shown in **Fig 3**a, two cross rulers were used to mark the FOV while the digital image sensor was used to obtain RGB (red, green, and blue) photographs. According to the training samples for supervised

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classification, neural network classification (NNC) was applied to classify the digital photos with ENVI 5.3 software[26], and this yielded the 3-EM classes (**Fig 3**b) and 4-EM classes (**Fig 3**c). The classification results were validated through visual interpretations. The observed endmember cover would not contribute equally to the ASD probe due to the point spread function (PSF) of the ASD sensor. Hence, it was necessary to calibrate the fractional cover.

The PSF is the Gaussian function, , where *d* is the distance from a pixel center (the unit is in meters) and σ illustrates the instantaneous FOV (IFOV) of a detector, which means that measurements closer to the center of the FOV will contribute more to the mixed reflectance signal, and thus, more weight should be given to the objects in the center. Each binary classified image was convolved with a Gaussian filter (i.e., *PSF* of the ASD sensor) to compute weighted averages of the image as shown in the **Fig 3**d. Endmember reference fractions could as such be expressed as a function of their actual contribution to the mixed pixel reflectance. Extensive research on this issue has been conducted by Settle [27] and Somers [28]. According to the PSF model, σ is 0.4363, which corresponds to a 25° IFOV for the ASD transformed to radians. Here, all the actual ground cover fractions were corrected to correspond to the PSF of the ASD sensor. In summary, all the classification images were convolved with a Gaussian filter, and then, the weighted average adjusted fractions of two photographs were taken as the reference fraction for the different endmembers in a plot.

Fig 3. NNC classification for 3-EM and 4-EM image and conversion techniques with the reference fractional cover. (a) Selected training sample. (b) Classified origin image for 3-EM. (c) Classified origin image for 4-EM. (d) 3D simulation of the Gaussian spread function applied on the classified images to give a representative weight corresponding to the pixel reflectance as measured by the spectral sensor. The weights sum to 1.

Data and Methods

Step 2.

Linear Spectral Mixture Model

In theory, linear spectral mixture modeling makes the physical assumption that each incident photon interacts with one earth surface component only, so the collected reflection spectra do not mix (i.e., no multiple scattering) before entering the sensor [29, 30]. We have constructed the LSMM (Eq. (1)) based on the principles of linear mixtures[13, 31-36]. The mixed spectra of the LSMM can be regarded as the linear combination of the endmember spectral response. In its general form, the LSMM can be described as follows:

(1)

where R_i is the measured reflectance of a mixed pixel in spectral band *i*; f_j is the sub-pixel cover fraction of the *j*th endmember in the pixel; and $W_{i,j}$ is the *j*th endmember reflectance for spectral band *i*; *m* is the number of the endmembers. Based on the measured pixel spectral vector R and the endmembers' spectral vector W, and this is done under the constraints that for j = 1, …, m (ANC) and (ASC). Since every pixel spectral, R, is acquired by spectral channels at different wavelengths, it can be represented by a column vector of which each component is a pixel in a plot. By making use of Eq. (1), the endmember fraction f_j estimates are obtained by the fully constrained least squares (FCLS) [37, 38] , for which the following equation is minimized:

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(2)

where n is the number of effective spectral bands; and. is the spectral model error. To impose the ASC, the linear mixing model is written as follows:

(3)

with , and a vector F by (4)

Here, is a parameter that weights the strength of the sum to one constraint; m is the number of the endmember.

The non-negatively constrained least squares (NCLS) impose the ANC on the abundance vector. The iteration algorithm proposed in [38] was adopted by introducing a Lagrange multiplier vector (λ) in Eqs. (5) and (6) to generate the solution:

(5)

(6)

Nonlinear Spectral Mixture Model

According to the characteristics of different NSMMs [39], this study proposes the use of a bilinear spectral mixture model (BSMM), which is relatively simple to use and yields results with physical meaning, and a kernel-based NSMM.

Bilinear Spectral Mixture Model

The bilinear spectral mixture models account for the presence of multiple photon interactions by introducing additional “interaction virtual” terms in the LSMM. Each term accounts for multiple interactions between endmembers and is represented by the cross-product of the interacting endmembers. BSMMs consider multi-order interactions between endmembers j and t (for j,t=1,…,m). Popular BSMMs include the Fan Model (FM)[40], Generalized Bilinear Model (GBM) [41], and Nascimento Model [42]. Considering the characteristics of *Nitraria* shrubs and *Haloxylon* structure in the study, we elected to use the Nascimento Model (Eq. (7)) without considering higher-order multiple scattering, i.e., we only considered the second order between endmembers and PV/NPV themselves as scattering.

(7)

where R_i is the measured reflectance of a mixed pixel in spectral band i, f_j is the sub-pixel cover fraction of the jth endmember in the pixel, $W_{i,j}$ is the jth endmember reflectance for spectral band i, $W_{i,j}W_{i,t}$ denotes the nonlinear combination of multiple scattering effects between endmembers, and ε_i is the spectral model error, $f_{j,t}$ describes the fraction of the tth second order mixture effects involving endmember j. The number of fraction products m is determined by that of the selected physical endmembers, and the number of fractions estimated includes all physical and virtual endmembers. By making ASC (sum to one constraint) and ANC (non-negativity constraint) constraints in the mixture model, and when $\forall\, j \geq t$, then $f_{j,t} = 0$, and when $\forall\, j < t$, then $f_{j,t} \geq 0$; meanwhile:

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and (8)

In Eq. (8), the virtual multiple scattering term is applied as additional endmembers. The FCLS algorithm is employed to unmixing $f_{j,t}$ and f_j , so $f_{j,t}$ is not related to f_j, which means they are separate. Because of the sum to one constraint (Eq. (8)) the 'virtual' fraction brings about significant underestimations of the actual ground cover, part of the interaction fraction $f_{j,t}$ should be assigned to each of the contributing physical entities[28]. The cover fraction f_j can easily be isolated from $f_{j,t}$ and estimated from Eq. (9) as :

(9)

where f_j is the fraction of the first-order interaction of endmember j, is the single scattering fraction, describes the fraction of the tth second-order mixture effects involving endmember j, and n is the number of the endmembers. The reader is invited to consult [17], [40]and [42] for more details.

Kernel-Based Nonlinear Spectral Mixture Model

1. **Kernel method**

The principle of the Kernel Nonlinear Spectral Mixture Model (KNSMM) is that the data from the input space R^N are mapped to the high-dimensional feature space H, through the implicit nonlinear mapping by kernel functions. By doing this, combinations of the original endmember spectral bands (i.e., some high-order multiplications of the original spectral bands) are now consisted of the components of each mapped endmember in the high-dimensional feature space. Therefore, the nonlinear mixture model is still linear and additive in the feature space but includes nonlinear components of the endmember spectral bands in the original input space [43-47].

Generally, the nonlinear mapping is unknown and may be complicated. Kernel-based learning algorithms use an effective kernel trick to implement dot products in feature space by employing some kernel functions[48]. The kernel representation for the dot products in H is expressed as:

(10)

Then everywhere that $x_i x_j$ occurs, we replace it with $K(x_i, x_j)$. Theoretically, any function that satisfies the Mercer's theorem[49, 50] or the Positive definite can be used as a kernel function. A Mercer Kernel is symmetric ($K(x_i, x_j) = K(x_j, x_i)$) and positive definite (($K(x_i, x_j) >0$)). By Mercer's theorem, any symmetric positive definite kernel represents the inner product in some higher-dimensional Hibert Space[50, 51]. According to the simple structure characteristics of the surface vegetation in the study area, we used two common kernel functions, namely, the radial basis function (RBF) kernel and the polynomial kernel function (PKF). The RBF and PKF were chosen due to their successful applications to non-linear unmixing in the scalar value case[46, 52]. RBF represents the case where an endless number of reflections occurs since it incorporates all higher order interactions between the input spectra, while PKF define the interactions order and has a relatively explicit physical meaning. The radial basis kernel function:

(11)

where σ is the parameter of the kernel function, and x_i and x_j are the spectral reflectance of endmember i and j. The polynomial kernel function :

(12)

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where *a*, *b*, and *c* are the parameters of the kernel function.

1. **Parameters of kernel function**

The optimal parameters in the RBF and PKF are determined by the minimum model unmixing RMSE. Because the training sample data is different for the different models and the different types of vegetation, the optimal parameters value of the kernel function is different. The parameter σ in the RBF is determined by the gradient descent method [53], and it was determined to 200 with the four endmember (4-EM) models and to 20 with the three endmember (3-EM) models in the *Nitraria* shrubs plots, and to 152 with the 4-EM models and to 200 with the 3-EM models in the *Haloxylon* plots. The parameters of PKF are determined by the Cross validation [54-57] which means that the fitting process optimizes the model parameters to make the model fit the input data as well as possible. The training data are split into *k* parts of size l/*k*. A discrete range of possible values of the kernel functions parameter is chosen and for each parameter value a spectral unmixing is trained using *k*-1 parts and tested on the remaining 1 part from which a model unmixing accuracy is measured since we know the labels of the data. This is repeated one by one through all *k* such splits of the training data into *k*-1 folds for training with testing on the remaining fold, and an average model unmixing accuracy is obtained. This is repeated for each of the parameter values and the value with the highest model unmixing accuracy is chosen. The polynomial order b = 2 was determined in the experiment, which refers to fourth-order statistical properties of the spectral data. a = 1/*n*, where *n* is the number of endmembers, and c = 1.

1. **Kernel fully constrained least squares (KFCLS)**

The KFCLS aims to find the abundance vectors via the objective function:

(13)

The KFCLS algorithm can be derived directly from the FCLS algorithm described in the previous section by replacing M^TM and M^TF used in the FCLS algorithm [44, 58]. Both of Eqs. (5) and (6) are kernelized by

(14)

(15)

It should be noted that $K(M, M)$ and $K(M, F)$in Eqs.(14) and Eqs.(15) are a kernel version of M^TM and M^TF, respectively. A detailed step-by-step implementation of KFCLS is available in[58], [59]and[60].We refer its derivations to these reference.

Accuracy Evaluation Model

In cases where accurate ground reference data are available, the quality of the sub-pixel abundance estimates can be assessed more reliably by checking the discrepancy between the estimated and reference endmember fractions. The spectral mixture model fit was checked by using the unmixing error of the spectral mixture model, the PV/NPV/BS/shadow ground validation RMSE (Eq. (16))[40], the R^2 (Eq. (17)) [7], and the Relative RMSE (RRMSE) (Eq. (18))[61]. The use of the RMSE of the spectral mixture model is mainly aimed at validating the accuracy of the model in unmixing the mixture

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spectral. The RMSE of endmembers was calculated to quantify the difference between the measured fraction and estimated fraction for the fields. RRMSE is a measure of the deviation rate with percent as the unit, and values closer to zero are indicative of a better fit. The relevant equations are as follows:

(16)

(17)

(18)

where RMSE is the root mean square error, R^2 is the square of the correlation coefficient, RRMSE is the deviation rate of the estimated model spectral value or estimated cover fraction of endmembers, n is the number of fields or available wavebands, x_i is the estimated cover fraction or the estimated mixing spectral value of the ith field, y_i is the measured cover fraction or measured mixing spectral value of the ith field, is the average value of the estimated cover fractions, and is the average value of the measured cover fractions.

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