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Analyzing the performance of PROSPECT model inversion based on different spectral information for leaf biochemical properties retrieval

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ABSTRACT

Leaf biochemical constituents provide useful information about major ecological processes. As a fast and nondestructive method, remote sensing techniques are critical to reflect leaf biochemistry via models. PROSPECT model has been widely applied in retrieving leaf traits by providing hemispherical reflectance and transmittance. However, the process of measuring both reflectance and transmittance can be time-consuming and laborious. Contrary to use reflectance spectrum alone in PROSPECT model inversion, which has been adopted by many researchers, this study proposes to use transmission spectrum alone, with the increasing availability of the latter through various remote sensing techniques. Then we analyzed the performance of PROSPECT model inversion with (1) only transmission spectrum, (2) only reflectance and (3) both reflectance and transmittance, using synthetic datasets (with varying levels of random noise and systematic noise) and two experimental datasets (LOPEX and ANGERS). The results show that (1) PROSPECT-5 model inversion based solely on transmission spectrum is viable with results generally better than that based solely on reflectance spectrum; (2) leaf dry matter can be better estimated using only transmittance or reflectance than with both reflectance and transmittance spectra.

1. Introduction

For understanding critical ecosystem processes, knowing species composition is almost as important as investigating the number of plant species (Hooper and Vitousek, 1997). Foliar biochemical properties such as chlorophyll, water, protein, cellulose, and lignin contents are important parameters connected to many biochemical processes, such as photosynthesis, evapotranspiration, respiration, and decomposing (Baldocchi, 1994; Ustin et al., 2009). Offering the advantage of being fast and nondestructive, remote sensing methods taking reflectance and transmittance spectra measurements became a general approach for researchers to study vegetation biochemical processes (Curran et al., 2001; Gitelson et al., 2006; Ustin et al., 2004).

Two remote sensing methods have been widely applied to retrieve leaf biochemical properties: the empirically-based model and physically-based model. The empirical model is often established by building vegetation indices from reflectance measurement and relating them to biochemical properties (Huete et al., 2002, 1997; Sims and Gamon, 2002; Zhao et al., 2013). This method is simple and convenient. Yet without a clear physical foundation, the performance of empirical models depends largely on the quality of training samples. It is also difficult for empirical relationships to be extended to different vegetation species and different locations (LaCapra et al., 1996; Martin and Aber, 1997). The physical model, on the other hand, simulates the process of radiation transmission and has good transferability. The parameters in a physical model have specific physical significance. The disadvantages of a physical model include that the number of parameters can be quite large, and building such a model is sophisticated and can involve complex computation (Jacquemoud et al., 2000; Sims and Gamon, 2002).

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A number of physical models have been proposed, such as PROSPECT (Jacquemoud and Baret, 1990; Jacquemoud et al., 1996), LIBERTY (Dawson et al., 1998), N-flux models (Allen and Richardson, 1968), stochastic model (Maier et al., 1999), and ray tracing models (Govaerts and Verstraete, 1998; Kumar and Silva, 1973). The development of radiative transfer models has shed light on the interactions between solar radiation and plant leaves. Among them, PROSPECT is widely used by the remote sensing community. It was proposed based on the plate model (Allen et al., 1969) and the version of PROSPECT-5 can accurately simulate the hemispherical reflectance and transmittance spectra of various plant leaves over the range from 400 to 2500 nm as a function of leaf structure index (N), leaf chlorophyll content (C_{ab}), leaf carotenoid content (C_{xc}), equivalent water thickness (EWT), and dry matter per area (LMA) (Feret et al., 2008). PROSPECT-D, the latest version, also included the calibrated specific absorption coefficient of anthocyanins to provide more insights on plant pigments (Féret et al., 2017).

Standard PROSPECT model inversion requires directional-hemispherical reflectance (hereafter referred to as R) and transmittance (hereafter referred to as T) spectra as model inputs. However, measuring both R and T is laborious and time-consuming. Traditional remote sensing techniques and methods mainly focus on the R spectrum, for the reflected echoes are easier to collect. As a result, many researchers omit the term of T in the merit function of PROSPECT model inversion, and retrieved leaf biochemical parameters with solely R spectrum (Li and Wang, 2011; Zhao et al., 2014).

Leaf transmission quantifies the amount of radiation attenuated through passing a leaf. The physical structure, as well as the biochemical constituents of a leaf (C_{ab}, EWT, etc.) influences the strength of this attenuation. Therefore, leaf T is closely connected to leaf constituents. With the new development of techniques and remote sensing methods, leaf T spectrum has been more and more available. For example, the ASD FieldSpec Pro FR (Analytical Spectral Devices, field spectroradiometer, full-range, Inc., Boulder, USA), some hand-held devices like the SPAD-502 (Markwell et al., 1995) or the N-Tester (Naud et al., 2009) provide rapid estimate of the light passing through the leaf at several wavelengths. High-resolution estimates of canopy transmittance (T_c) are also significant in many environmental applications (Milenković et al., 2017). As a result, though current sensors mounted on air or space mainly focus on collecting reflected signals, many studies are devoted to estimate T_c using new technologies and methods (Oshio and Asawa, 2016; Parker et al., 2001; Solberg et al., 2006). For example, LiDAR returns can be analyzed for T_c (Ma et al., 2017; Morsdorf et al., 2006). This study investigates the PROSPECT model inversion strategy based solely on T spectrum. As comparisons, the results with R only and both R plus T have also been analyzed. The performance comparison will help researchers make decisions while making measurement strategies.

In this study, we (1) generated synthetic R and T spectra (with varying levels of random and systematic noise) considering the correlations between leaf biochemical parameters with PROSPECT-5, and used the synthetic dataset to compare the performance of three inversion strategies: T, R and R plus T; (2) analyzed the influence of random and systematic errors in R and T spectra on model inversion performance using the synthetic dataset; and (3) analyzed the performance of the inversion strategy using T spectrum by comparison with the strategies of R and R plus T spectra using two independent experimental datasets: LOPEX and ANGERS. Biochemical concentration predicted from model inversion is compared with measured biochemical composition. Direct comparison between simulated and measured R (and T) is used to assess the performance of the models in terms of accuracy of fit.

2. Materials and methods

2.1. Data description

2.1.1. Design of a synthetic dataset

To make a comprehensive test on the model's inversion performance with T, R and R plus T, a large volume of spectral data and the corresponding leaf biochemical contents are needed. The experiments in this study were conducted on two types of datasets: the simulated synthetic dataset and the experimental dataset.

Before running the PROSPECT model in the forward mode, the calibration procedure of several important parameters (the refraction index and the specific absorption coefficients of leaf constituents) is often needed. The two steps were followed as in Feret et al. (2008), benefiting from leaf samples in ANGERS. The calculated refraction index and specific absorption coefficients were close to those in PROSPECT-5. As a result, PROSPECT-5 was directly used in leaf spectra simulation and leaf traits inversion.

Running PROSPECT-5 in the forward mode can generate a large synthetic spectral dataset by incorporating a wide range of parameters and variability (Morsdorf et al., 2009). In this study, the leaf constituent ranges of variation, the means and standard deviations for C_{ab}, C_{xc}, EWT and LMA were similar to Féret et al. (2011)'s. The means and standard deviations (Std.) of N were calculated from the datasets LOPEX and ANGERS (Table 1). The close relations between C_{ab} and C_{ab} ($R^2 = 0.86$), LMA and EWT ($R^2 = 0.63$) were considered here. Assuming that all the parameters follow Gaussian distributions based on Table 1, a total of 500 leaf constituents' combinations were generated where all parameters vary at the same time. This sampling scheme can largely diminish the number of simulations needed, compared with uniform random drawing. Additionally, the size of dataset in this study was settled based on Féret et al. (2011)'s study, who found that a dataset containing 500 samples led to similar results to a larger dataset with 2401 samples, both using the method of design of experiment. Thus, by running PROSPECT-5 model in the forward direction, 500 R and T spectra make up the synthetic dataset.

In order to test the model inversion performance against random noises and consider possible sensor calibration errors, random noise and systematic noise have been added on spectra of the synthetic dataset. Firstly, additive random Gaussian noise with standard deviation (std.) of the same level (3%, 7%, 10%) of R and T amplitudes was applied on every wavelength of R and T spectra, respectively. Secondly, a relative bias (5%, 10%, 15%) was added to produce the final synthetic dataset.

2.1.2. Description of the experimental datasets

In order to take the various realistic factors in actual measurements into consideration, and validate the inversion results with synthetic dataset, we have compiled two independent experimental datasets. The first is Leaf Optical Properties Experiment (LOPEX) dataset (Hosgood et al., 1995), which was established by the Joint Research Center of the European Commission in 1993. The version utilized was updated on 9 March 2015. This dataset includes 45 different species, 320 fresh leaf samples. The second is ANGERS leaf optical properties database (Feret et al., 2008), which was established by S. Jacquemoud etc. in June 2003, Angers in France. This dataset includes 43 different species, 276 leaf samples.

LOPEX and ANGERS datasets encompass altogether 596 leaves of woody and herbaceous species, representing a large variety of leaf internal structure, biochemical composition and spectrum. In both datasets, leaf R and T spectra were measured in the optical range (1-nm steps) with laboratory spectrophotometers or field spectroradiometers equipped with integrating spheres. In this study, we selected four biochemical parameters expressed in the