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PROCWT: Coupling PROSPECT with continuous wavelet transform to improve the retrieval of foliar chemistry from leaf bidirectional reflectance spectra

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ABSTRACT

The leaf optical properties model PROSPECT has been widely used to retrieve foliar chemistry in reverse mode from directional-hemispherical reflectance factor (DHRF) spectra measured with integrating sphere equipped spectrometers. With bidirectional reflectance factor (BRF) spectra, some researchers attempted to invert PROSPECT after a modification to the latest version of the model. However, the retrieval accuracy varies greatly with chemical constituents and can be low for some of them, such as dry matter content. This paper proposes a new approach called PROCWT by coupling PROSPECT with continuous wavelet transform (CWT) to suppress the surface reflectance effect and enhance the absorption features of chemical constituents. Instead of the reflectance spectra, the wavelet coefficient spectra generated after CWT were used to construct the merit function for model inversion. Given that the multi-scale decomposition of CWT enables enhancement of chemical-specific absorption features, the use of PROCWT at different scales of wavelet decomposition could lead to improved retrievals of biochemical parameters. The performance of PROCWT was evaluated for estimating foliar chemicals of wheat and rice crops from BRF spectra measured with a leaf clip equipped spectrometer over a two-year field experiment. PROCWT was also compared with the standard PROSPECT inversion (STANDARD), the PROSPECT inversion with the subtraction of surface reflectance (PROREF), and the simplified PROCOSINE (sPROCOSINE).

Our results demonstrated that the contribution of surface reflectance component was significant for BRF spectra and the effect of surface reflectance could be suppressed by PROCWT as well as PROREF and sPROCOSINE. Compared with STANDARD, PROCWT and the two traditional methods significantly improved the retrieval accuracies for pigments and leaf water content, but only PROCWT produced significant improvement for dry matter content with a decrease of 14.79 g/m^2 in the root mean squared error (RMSE) (30% of the mean) over the entire experimental dataset by enhancing dry matter absorption features. High scales of wavelet decomposition were favorable for the estimation of carotenoid and water contents and low scales for the estimation of chlorophyll and dry matter contents. The difference in optimal scale revealed the separation of overlapping absorption features attributed to various chemical constituents. In addition, the newest PROSPECT-D outperformed PROSPECT-5B in the retrieval of chlorophyll content but not for carotenoid. This new physically-based approach could be beneficial to analysts attempting to retrieve leaf chemicals from BRF spectra alone and close-range reflectance imagery of crops and even other vegetation types.

1. Introduction

Wheat and rice are two major staple crops in the world and provide primary food for more than half of global population (Seck et al., 2012; Shiferaw et al., 2013). Quantifying the foliar chemical constituents of these crops could provide valuable information for better understanding plant physiology (Gamon and Surfus, 2010), practicing precise farming (Haboudane et al., 2002) and implementing plant phenotyping (Yendrek et al., 2017). As one of the most important pigments, chlorophylls (chlorophyll *a* and *b*, denoted as C_{ab}) absorb light energy for photosynthesis (Anderson, 1986; Demmig-Adams and Adams, 1992) and are closely related to the nitrogen content (Evans, 1989), which is a valuable indicator for agronomists to make fertilization recommendations (Li et al., 2016). In addition, carotenoids (C_{xc}) are important accessory pigments during photosynthesis process for their roles in photoprotection under high irradiance levels (Ritz et al., 2000). Besides

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photosynthetic pigments, leaf dry matter content (C_m) is a key trait in light capture and plant growth (Kattge et al., 2011) and leaf water content (C_w) is a useful indicator for irrigation management (Ben-Gal et al., 2009) and freezing injury detection (Wei et al., 2017).

Remote sensing of these foliar chemicals is often performed using two approaches: empirically-based and physically-based (Féret et al., 2017). The common practice for the former approach is to establish linear or nonlinear relationships between foliar chemicals and spectral parameters, such as widely used vegetation indices (Féret et al., 2011) and wavelet features (Cheng et al., 2014b). However, these empirical relationships often need to be recalibrated when applied to a new dataset, thereby leading to the lack of transferability and robustness (Li and Wang, 2011; Féret et al., 2017). The physically-based approach is based on radiative transfer models by which the leaf chemicals are inversely retrieved from spectral data (Jacquemoud and Baret, 1990). Compared with the empirically-based one, the physically-based approach is more generic and robust because the physical models can be directly applied to new datasets (Féret et al., 2008). PROSPECT, developed by Jacquemoud and Baret (1990) more than two decades ago, is the most popular leaf optical properties model due to its ease of use, generalization capability and free access (Jacquemoud et al., 2009). Until now, several versions of the model have been released and the newest version PROSPECT-D for the first time allows three pigments (C_{ab}, C_{xc} and C_{anth}) to be inverted simultaneously (Féret et al., 2017).

In the past two decades, many studies have reported on the successful retrieval of foliar chemicals by PROSPECT with directional-hemispherical reflectance factor (DHRF) and transmittance (DHTF) spectra measured with integrating sphere equipped spectrometers (Table 1). Some researchers also inverted PROSPECT with leaf bidirectional reflectance factor (BRF) and transmittance factor (BTF) spectra measured with leaf clip equipped spectrometers, which are easier and more efficient to operate than those with integrating spheres (Li and Wang, 2011; Ma et al., 2012; Zhang and Wang, 2015). However, the PROSPECT models do not apply well to BRF spectra (Jay et al., 2016) because they were originally calibrated on DHRF and DHTF spectra instead of BRF and BTF spectra (Jacquemoud and Baret, 1990; Féret et al., 2008). This problem may be attributed to the difference in physical property between DHRF and BRF spectra. Firstly, leaves are not Lambertian and hence leaf reflectance exhibits anisotropy properties (Bousquet et al., 2005), which makes leaf BRF measurements sensitive to the view angle. Secondly, both DHRF and BRF spectra contain the diffuse component and the surface component because part of light does not penetrate into the leaf and bounces off the leaf surface directly (Jay et al., 2016). Although the surface reflectance is minimal (even negligible in some cases) for the DHRF at nadir illuminations (Walter-Shea et al., 1989; Bousquet et al., 2005), the contribution of surface reflectance may be significant for the BRF measured in the same illumination condition (Sims and Gamon, 2002; Comar et al., 2012). This imposes adverse effects on the subsequent model inversion and hence limits the application of PROSPECT to the BRF spectra measured with the leaf clip assembly and close-range imaging spectroscopy systems (Jay et al., 2016).

To cope with the retrieval from BRF spectra, one could separate the surface reflectance from the diffuse reflectance because only the latter, resulting from the interaction process within the leaf mesophyll, is useful for quantifying leaf chemical constituents (Bousquet et al., 2005). The surface component may be measured directly with polarization photometers (Vanderbilt and Grant, 1986), but these devices are complex to operate and not commonly used for such a purpose. As an alternative approach, Bousquet et al. (2005) proposed a three-parameter physical model to simulate leaf surface reflectance, but this model is overparameterized and difficult to be used in practical applications. Recently, Jay et al. (2016) proposed a physically-based method called PROCOSINE to account for the effect of surface reflectance and leaf orientation and successfully retrieved foliar chemicals from close-range imaging spectroscopy data. Although the application of PROCOSINE to reflectance spectra can remove the effect of surface reflectance, the retrieval accuracy varies greatly with chemical constituents and remains to be improved for some of them, such as C_m.

Among all leaf chemicals, C_{ab} and C_w are the most extensively investigated with satisfactory retrieval accuracy (Gitelson et al., 2003; le Maire et al., 2004; Maki et al., 2004) because of their strong absorption features in leaf reflectance spectra (Féret et al., 2011). Quantifications of C_{xc}, C_{anth} and C_m are much more challenging because their absorption features are masked by C_{ab} in the visible region and C_w in the shortwave infrared (SWIR) region (Gitelson et al., 2002; Gitelson et al., 2009; Cheng et al., 2014b). To improve the retrieval accuracy, researchers have proposed various strategies, such as stepwise inversion (Li and Wang, 2011), optimization of spectral regions (Wang et al., 2015b) and exploitation of a priori information on model input parameters (Ali et al., 2016). However, the improvements are still limited, especially for C_m with weak absorption features in the SWIR region. A simple method that can enhance the absorption features and remove the effect of surface reflectance is desired for retrieving these chemical constituents from BRF spectra.

Recently, continuous wavelet transform (CWT) has been used in some studies to estimate C_{ab} (Blackburn and Ferwerda, 2008), C_w (Cheng et al., 2011) and C_m (Cheng et al., 2014b) from hyperspectral data. CWT decomposes a leaf reflectance spectrum into a number of scale components through a mathematical transformation. Each component has the same length as the reflectance spectrum (Cheng et al., 2011) and is composed of wavelet features or wavelet coefficients as a function of wavelength and scale. The multi-scale decomposition of CWT could help identify the absorption features more accurately than traditional spectral index based methods (Cheng et al., 2014b). Narrow absorption features in the original reflectance spectrum are captured at a low decomposition scale while the broad ones are captured at a high scale (Rivard et al., 2008; Ullah et al., 2012). However, existing studies only made use of a small number of wavelet features for empirically-based methods (Blackburn and Ferwerda, 2008; Ullah et al., 2012; Cheng et al., 2014b) and none of them has investigated the application of CWT in physically-based methods. Coupling PROSPECT and CWT has the potential to improve the retrieval of leaf chemistry by enhancing their absorption features. In addition, we hypothesize that the linear additive property of CWT (Rivard et al., 2008) could suppress the effect of surface reflectance and make PROSPECT model inversion applicable to BRF spectra. Therefore, the objectives of this study were (1) to propose a wavelet-based PROSPECT inversion method called PROCWT by coupling PROSPECT with CWT to reduce the surface reflectance effect and enhance the absorption features of chemical constitutions, and (2) to evaluate the performance of PROCWT and compare it to three inversion methods in terms of the retrieval of leaf chemistry for rice and wheat crops.

2. Materials and methods

2.1. Experimental design

Four experiments were conducted for field sampling over two consecutive years at the experimental station in Rugao, Jiangsu of eastern China (120°45′E and 32°16′N). The treatment in each experiment encompassed a combination of cultivar, nitrogen fertilization rate and planting density for wheat and rice in rotation cropping which is a typical farming system for this area (Table 2). A split plot design with three replications was used for all experiments and each plot was in the same size of 5 m × 6 m. Wheat was sowed in drill and the rows were oriented in a south-north direction with different row spacings. Rice was grown in a grid pattern with a plant spacing of 15 cm and two row spacings of 30 and 50 cm. Field sampling for the wheat and rice seasons of 2015 was performed at the stages of jointing, booting and heading. Sampling in the seasons of 2016 was only conducted at jointing and booting. The experimental data from 2015 and 2016 for wheat and rice