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Different units of measurement of carotenoids estimation in cotton using hyperspectral indices and partial least square regression

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ABSTRACT

This paper examines the use of canopy reflectance for different units of measurements of carotenoids estimation. Field spectral measurements were collected over cotton in different intensive field campaigns organized during the growing seasons of 2010 and 2011. Three units of measurement were evaluated carotenoids expressed as a mass per unit soil surface area (g/m^2), a mass per unit leaf area (μg/cm^2), and a mass per unit fresh leaf weight (mg/g), respectively. Four methods were compared to retrieve amount of carotenoids: stepwise multiple linear regression (SMLR), published spectral indices, band combination indices, and partial least square regression (PLSR). Results show that maximum sensitivity of reflectance to variation in different units of measurement of carotenoids was found in the green region at 515–550 nm, and at 715 nm and 750 nm regions in the far-red wavelengths. The predictive accuracies of Car (g/m^2), Car (μg/cm^2) and Car (mg/g) were tested on a validation data set and the results show that the highest R^2 values between estimations and observations were 0.468 for Car (g/m^2), 0.563 for Car (μg/cm^2), and 0.456 for Car (mg/g), with relative root mean square error (RMSE%, RMSE/mean) of 48.72%, 22.07% and 21.07%, respectively. Compared to Car (g/m^2) and Car (mg/g), the model performance indices for Car (μg/cm^2) show a high degree of consistency among the R^2 values and RMSE% and MAE% values. Further comparison were performed among the estimation accuracies of different unit carotenoids and among the different approaches used in the study by a paired-*t*-test. The results indicate that although the best estimation results for Car (μg/cm^2) and Car (mg/g) were both obtained based on PLSR, they can be estimated by all four adopted methods without significant differences ($P > 0.1$). Whereas for Car (g/m^2), the best estimation results were obtained based on published vegetation indices CIred-edge, which were significantly better than the estimation results based on SMLR ($P < 0.000$). In summary, the results of this study show that even the carotenoids expressed on concentration (mg/g) or content (μg/cm^2) basis at leaf level can be estimated with the same prediction accuracies to the carotenoids expressed as a mass per unit surface area (g/m^2) at canopy level using reflectance measurement at canopy level.

1. Introduction

Remote sensing techniques are a prominent tool for determining the plant physiological state (Zur et al., 2000). Leaf chemical constituents are determining indicators of plant physiology and other functional processes up to the ecosystem level. Among them, plant pigments are the most studied traits (Blackburn, 2007; Ustin et al., 2009). Carotenoids (Car) and chlorophylls (Chl) are the main pigments of green leaves (Gitelson et al., 2002). Measurement of total chlorophyll content (Cab) and carotenoids content (Car) has many applications in agriculture, ecology, and Earth science. The methods for remote estimation of chlorophylls a and b (Cab) have been quite well established (Gitelson et al., 2009; Haboudane et al., 2002; Le Maire et al., 2004, 2008; Malenovský et al., 2013; Schlerf et al., 2010; Zarco-Tejada et al., 2004), However, for carotenoids (Gitelson et al., 2002, 2006; Hernández-Clemente et al., 2012), are still not well developed.

Carotenoids are also important photosynthetic pigments (Demmig-Adams and Adams, 1992). Carotenoids have several physiological functions associated with photosynthesis, including structural role in the organization of photosynthetic membranes,

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participation in light harvesting, energy transfer, as well as quenching of Chl excited states and photoprotection (Demmig-Adams et al., 1996; Edge et al., 1997; Horton et al., 1996; Peterman et al., 1997; Young and Frank, 1996).

During the last decade, some attempts have been undertaken to develop nondestructive techniques for Car assessment (Asner and Martin, 2008; Blackburn, 1998, 1999; Chappelle et al., 1992; Datt, 1998; Féret et al., 2008; Gitelson et al., 2002, 2006; Sims and Gamon, 2002; Thomas and Gausman, 1977; Zur et al., 2000). In these studies, different units have been used to express amounts of carotenoids, e.g. nmol/cm^2 (Gitelson et al., 2002), mg/cm^2 (Datt, 1998), μg/cm^2 (Hernández-Clemente et al., 2012; Zarco-Tejada et al., 2013). Data has been expressed in units of area, or mass. The most common three units of measurement were evaluated cartenoids expressed as a mass per unit surface area (g/m^2), a mass per unit leaf area (μg/cm^2), and a mass per unit fresh leaf weight (mg/g). These three units of measurement are different but are often used in remote sensing.

Grossman et al. (1996) showed that band selection using stepwise multiple linear regression, depended on whether the chemical data were expressed on a concentration (g/g) or content (g/m^2) basis. For a given chemical, similar bands were selected on a concentration or a content basis less than 6%. Datt (1998) indicated that the use of content (a mass per unit leaf area) rather than concentration (a mass per unit leaf mass) has been found to be more suitable for remote sensing applications because it is a better representation of amount of matter interacting with light per unit surface area. Furthermore, literatures also demonstrated that in order to be compatible with remotely sensed canopy reflectance, the leaf level chemical measurements were normally multiplied by biomass or LAI to be upscaled to the canopy level, and the canopy properties were expressed as a mass per unit surface area (g/m^2) (Homolová et al., 2013). However, it still remains unclear how significant differences are when a chemical expressed on concentration (mg/g) or content (μg/cm^2) basis at leaf level was estimated using reflectance measurement at canopy level, and few efforts have been made for comparing the accuracy of a chemical estimation based on different unit expressions, concentration (mg/g), content (μg/cm^2) and density (g/m^2), using experimental canopy reflectance measurement.

Some previous studies have compared retrieval capability for a given unit measurement of chemical at different remote sensing scales. For instance, Bian et al. (2013) have established the relationships between the concentrations (mg/g) of some key biochemical compounds of tea and the reflectance at three different levels: powder, fresh leaf and canopy levels. But until now, the relationships between the different units of measurement of carotenoids or any other biochemical compounds and the reflectance measurement at a given level (canopy-level in this study) have not been well discussed.

Additionally, most of the algorithms or vegetation indices for carotenoids reported in these literatures have been developed using leaf reflectance measurements carried out on a few deciduous and coniferous species from the northern hemisphere (Hernández-Clemente et al., 2012; Zarco-Tejada et al., 2013). Such algorithms and vegetation indices need to be applied to other species from different geographical and climatic regions of the world to see if they are indeed general. The cotton in Xinjiang, China, is different from the vegetation types usually described in remote sensing literature for carotenoids, where carotenoids content and chlorophyll content are relatively higher than forest sites. Furthermore, the continental arid climate of Xinjiang is characterized by aridity, rich sunlight and rare rainfall. The previous studies have proved that the photoprotection system plays a critical role in plants adapted to high temperature, high irradiation levels and drought (Faria et al., 1996; Hernández-Clemente et al., 2011). Very few high spectral resolution reflectance studies been carried out on cotton in China, and none of these have investigated the relationships between canopy reflectance and amount of carotenoids. This study is the first to investigate, in detail, the relationship between different units of measurement of carotenoids and experimented canopy reflectance measurement for cotton.

The present study investigated the relationship between cotton canopy reflectance measurement and the amounts of carotenoids by comparing carotenoids expressed as a mass per unit area (Car (g/m^2) and Car (μg/cm^2)) and as a mass per unit mass (Car (mg/g)) using stepwise multiple linear regression (SMLR), published vegetation indices, band selection indices and partial least square regression (PLSR) approaches. The main aims of the study were (1) to analyze the relationships between canopy hyperspectral reflectance and different units of measurement of carotenoids; (2) to compare the estimation accuracy of the different units of measurement of carotenoids; (3) to assess the prediction capability of SMLR, published vegetation indices, band-selection indices and PLSR in different units of measurement of carotenoids estimation.

2. Material and methods

2.1. Field data collection

The field experiment was conducted in June–September 2010 and 2011 at agricultural belts in Shihezi, Xinjiang, Northwest of China (85°59′E, 44°19′N), where cotton is the dominate crop. The continental arid climate of Xinjiang is characterized by aridity, rich sunlight and rare rainfall, with sharply defined seasons, high annual and diurnal fluctuations in air temperature, and low precipitation. Cotton is generally planted in April–May, and harvested in September–October. The whole growth period is about 180 days. The medium loam soil at the experiment area had the following properties: the field moisture capacity at depth of 10 cm was 0.33 g/cm^3, the volumetric water content at depth of 10 cm was 1.59 g/cm^3, and the saturation moisture content was 0.44 g/cm^3.

Field data collection were conducted in June–September 2010–2011 for eight times from seedling stage until boll stage (the actual dates were 12 June, 14 July, 8 August, and 8 September, 2010; 24 June, 11 July, 28 July, and 17 August, 2011, respectively). This procedure ensured that the normally occurring variation due to growth stage and measurement factors was included in the models, giving a more realistic basis for model development.

Canopy reflectance was obtained using an Analytical Spectral Devices, FieldSpec Full Range (ASD FieldSpec FR, Analytical Spectral Devices, Inc., Boulder, CO, USA) that acquires continuous spectra from 350 to 2500 nm. All canopy spectral measurements were taken on clear days with no visible cloud cover between 10:00 am and 14:00 pm (Beijing local time) since during this period the weather conditions and sunlight conditions were generally at the most stable state. In each plot, representative plants were selected for canopy spectral measurement. Taking into account the impact of soil background, in the first field campaign, the sensor head was placed about 0.3 m vertically above the canopies. This resulted in a spot size of 13 cm in diameter in each measurement since the ASD sensor has a field of view of 25 degrees. In the other field campaigns, the sensor head was placed approximately 1 m vertically above the canopies, leading to a spot size of approximately 44 cm in diameter on the canopies.

The reflectance of a white Spectralon panel (BaSO4) was measured before every reflectance was taken, then the reflectance was calculated as the ratio between energy reflected by the canopy and energy incident on the canopy. Every reflectance was an average of ten repeated scans that were automatically acquired by the FieldSpec.