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Retrieval of leaf biochemical properties by inversed PROSPECT model and hyperspectral indices: an application to *Populus euphratica* polymorphic leaves

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Abstract: Leaf biochemical properties have been widely assessed using hyperspectral reflectance information by inversion of PROSPECT model or by using hyperspectral indices, but few studies have focused on arid ecosystems. As a dominant species of riparian ecosystems in arid lands, *Populus euphratica* Oliv. is an unusual tree species with polymorphic leaves along the vertical profile of canopy corresponding to different growth stages. In this study, we evaluated both the inversed PROSPECT model and hyperspectral indices for estimating biochemical properties of *P. euphratica* leaves. Both the shapes and biochemical properties of *P. euphratica* leaves were found to change with the heights from ground surface. The results indicated that the model inversion calibrated for each leaf shape performed much better than the model calibrated for all leaf shapes, and also better than hyperspectral indices. Similar results were obtained for estimations of equivalent water thickness (EWT) and leaf mass per area (LMA). Hyperspectral indices identified in this study for estimating these leaf properties had root mean square error (RMSE) and R^2 values between those obtained with the two calibration strategies using the inversed PROSPECT model. Hence, the inversed PROSPECT model can be applied to estimate leaf biochemical properties in arid ecosystems, but the calibration to the model requires special attention.

Keywords: *Populus euphratica*; inversed model; hyperspectral index; vertical profile; polymorphic leaf

Leaf biochemical properties indicate the growing status of natural vegetation and crops and are the main input variables of many ecological models. Because biochemical properties determine the spectral reflectance of leaves and canopies, leaf biochemical properties hence can be studied via reflectance and *vice versa*. Remote study of leaf biochemical properties by measuring reflectance from various platforms has become an important tool for understanding the functioning of terrestrial ecosystems. Currently, there is a growing interest in hyperspectral remote sensing for research and application in a variety of fields including geology, agriculture, forestry, coastal and inland water studies, assessment of environment hazards, and urban studies (Zhao *et al.*, 2005).

Two main approaches are generally used to measure

leaf biochemical properties with hyperspectral remote sensing: model inversion and indices. As for model inversion, many physically based models have been developed to simulate leaf reflectance spectra and estimate leaf biochemical parameters and *vice versa*. Currently, PROSPECT is the most popular and simple inversion model because it can accurately simulate the hemispherical reflectance and transmittance of various plant leaves over the solar spectrum from 400 to 2,500 nm (Jacquemoud and Baret, 1990). It has been successfully used in many studies to retrieve leaf chlorophyll contents (Chl) and water and dry matter contents for a large number of broadleaf species (Zarco-Tejada *et al.*, 2002).

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The use of hyperspectral indices, although not as theoretically based as the use of model inversions, offers two main advantages. First, the most informative wavelengths in the whole domain can be selected, and second, a narrow spectrum feature can be used to assess the biochemical properties of the vegetation (Broge and Mortensen, 2002). In addition, the indices are easier to use than model inversions. Many studies have documented that hyperspectral measurements can be used to quantify biophysical characteristics of vegetation at leaf scale (Gitelson *et al.*, 2003) or canopy using *in situ*, airborne (like AVIRIS, CASI and HyMap) or spaceborne data (like Hyperion and CHRIS). Le Maire *et al.* (2004) identified various types of indices for retrieving broadleaf chlorophyll content and calibrated the wavelengths of these indices on a large simulated database to obtain the best possible index for each type.

Although both approaches have been applied in various ecosystems, neither approach has been used to estimate leaf biochemical properties in arid ecosystems based on hyperspectral data. This is largely because the reflectance data from vegetation in arid ecosystems are weak and not very different from reflectance data from the nonvegetated background. Ecosystems in arid lands, however, are extremely fragile and quite sensitive to climate change and human activities. For these reasons, arid lands are currently receiving increasing attention from researchers.

Populus euphratica is an important tree species in arid lands. More than 60% of the world's *P. euphratica* forests are in China, with 91.1% of them in the Tarim River Basin in Xinjiang, covering an area of $3.52 \times 10^5 \text{ hm}^2$ (Wang *et al.*, 2002). It is one of the oldest species of the original desert riparian ecosystem and is important for conserving and improving the ecology and environment in arid areas, such as the lower reaches of the Tarim River. Unlike other tree species, *P. euphratica* produces polymorphic leaves, i.e. leaf shape varies with growth stage and height in the canopy.

In this study, we indirectly estimated leaf biochemical properties using both model inversion and hyperspectral indices for the polymorphic leaves of *P. euphratica* in arid lands. The first objective was to evaluate the applicability of the inversed PROSPECT model in arid ecosystems, which has been widely ap-

plied to non-arid ecosystems. Because the different kinds of *P. euphratica* leaves are generally distributed at different heights along the vertical axis of the canopy, the study will not only provide extensive validation of the inversed PROSPECT model but also provide useful insights for upscaling, e.g., for canopy-scale reflectance simulation. The second objective of the study was to determine hyperspectral indices for leaf biochemical properties of plants in arid ecosystems, which included chlorophyll content (Chl), equivalent water thickness (EWT), and leaf mass per area (LMA). Reflectance spectra and biophysical/biochemical properties along the vertical axis of *P. euphratica* canopies were measured at Aragan region in the lower reaches of the Tarim River.

1 Materials and methods

1.1 Study area

The Tarim River is the longest inland river in China, and the "Green Corridor" dominated by *P. euphratica* forests is located in its lower reaches between the Taklimakan Desert (the second largest mobile desert in the world) and the Kumtagh Desert. *P. euphratica* community propagation conserves the ecology and environment in the lower reaches of the Tarim River (Ma *et al.*, 2009). The *P. euphratica* canopies at Aragan region in the lower reaches of the Tarim River were measured in this study.

In the study area, the average annual temperature is 10.8°C , the average range in daily temperature difference 16.7°C , and the annual accumulated temperature of $\geq 10^\circ\text{C}$ ranges from $4,169^\circ\text{C}$ to $4,218^\circ\text{C}$. The annual total solar radiation, sunshine duration, and frost-free period are $6,180 \text{ MJ/m}^2$, 3,000 hours, and 175–195 days, respectively. The precipitation is low (only 17 mm to 34 mm annually), but the annual potential evaporation can be as high as 2,408–2,671 mm, making the Tarim River Basin one of the most arid areas in China. Sandstorms and drifting dust occur frequently. The prevailing wind directions are east and southeast, with the main wind season from March to June. In addition, gales and dry-hot winds occur frequently during the periods from April to May and from June to August. According to the statistical data, gale winds ($> 17 \text{ m/s}$) occur 6.7 days per year on average. The dominant vegetation species in the study area are *P.*

euphratica and *Tamarix* sp. Both of these species grow at the banks along the river channel.

1.2 Leaf sampling and measurements

Along a transect perpendicular to the river channel, six typical mature *P. euphratica* trees with different distances from the river channel were randomly selected (Fig. 1). To investigate the variation of biophysical and biochemical properties of *P. euphratica* polymorphic leaves along the canopy vertical axis, about 100 leaves were sampled in each tree at 1-m intervals from the bottom to the top. Leaf reflectance and transmittance of the removed leaves were measured *in situ* using a spectroradiometer (ASD FieldSpec FR, ASD, USA) equipped with a leaf clip. After spectra were collected, fresh weights were measured and leaf areas were scanned, all samples were immediately frozen in liquid nitrogen and stored at -80°C for later chlorophyll-extraction in the laboratory. Chlorophyll was extracted with an 80% aqueous acetone solution and then centrifuged before being measured with a spectrophotometer (Beckman DU800) for absorption spectra. The concentrations of chlorophyll a and b were calculated from the absorbance measured at 646.6, 663.6 and 730 nm according to the Porra formula (Porra *et al.*, 1989). Leaf water content was determined from the weight loss after 12 hours in a fan oven at 70°C . All samples were scanned with a scanner to calculate leaf areas. The equivalent water thickness and dry matter weight were then calculated as follows:

$$\text{EWT} = (\text{Wf} - \text{Wd}) / A, \quad (1)$$

$$\text{LMA} = \text{Wd} / A. \quad (2)$$

Where EWT is the equivalent water thickness (g/cm^2), Wf the fresh weight, Wd the dry weight, A the leaf area, and LMA the leaf mass per area (g/cm^2).

1.3 PROSPECT model calibration and inversion

The PROSPECT model is a simple radiative transfer model in which a plant leaf is regarded as a succession of absorbing layers. This model has been widely used to simulate the leaf directional-hemispherical reflectance and transmittance from 400 to 2,500 nm. Because it requires only a small number of input variables and therefore can be readily inverted (Schaeppman-Strub *et al.*, 2006), the PROSPECT model has been inverted to

estimate leaf biochemical properties (Riaño *et al.*, 2005; Colombo *et al.*, 2007). Before the PROSPECT model is inverted, physical and optical constants, such as the refractive index of leaf material $n(\lambda)$, must be calibrated with experimental data (Feret *et al.*, 2008).

If the PROSPECT model is used to simulate the biochemical constituents of all leaves of *P. euphratica* growing in arid areas, the errors would be large. The particular polymorphic leaves of *P. euphratica* grow under extremely arid environments, and both shape and internal structure of the polymorphic leaves are different (Yang *et al.*, 2005; Zheng *et al.*, 2006; Yue *et al.*, 2009). Therefore, we calibrated the model so as to derive more veracious simulated results. However, the errors of biochemical constituents of the mixed leaves, simulated with the calibrated model, are still large. Thus, the biochemical constituents of three types of leaves are separately simulated. For the hyperspectral indices, some waveband combinations can be used to estimate the biochemical constituents of all leaves, so there is no need to find indices for separate types of leaves.

PROSPECT-5 and PROSPECT-4 are both published by Feret *et al.* (2008), and the processes for Cw and Cm are completely the same in their source code. The parameter of carotenoid was added in PROSPECT-5,

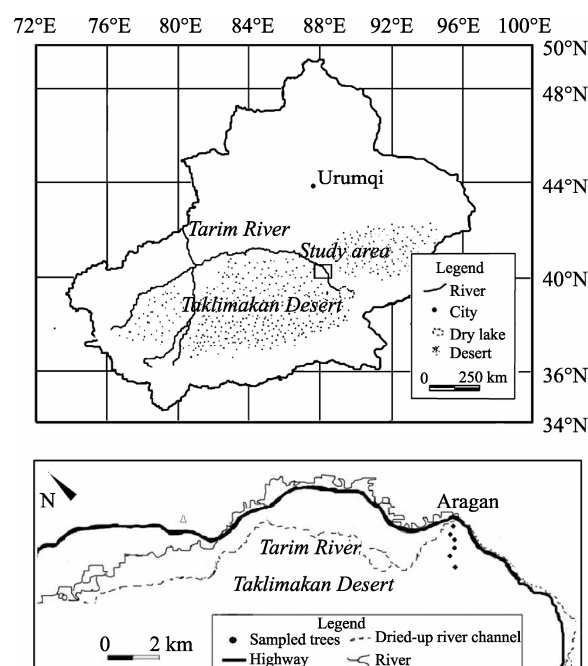


Fig. 1 Geographical location of the study area

which results in a small difference of the extinction coefficient of Cab at 400–600 nm. We did not measure the values of carotenoid content, however, carotenoid is not the main pigment in *P. euphratica* leaves, and its content is very low at the peak growth stage of *P. euphratica* leaves. Therefore, the contents of chlorophyll in *P. euphratica* leaves were measured instead of carotenoid content in this study, and PROSPECT-4 was inversed to estimate Chl, EWT and LMA. The calibration and inversion of PROSPECT-4 followed the procedures of Feret *et al.* (2008). The calibration stage aims at assessing the refractive index $n(\lambda)$ and the specific absorption coefficient $k_{spe}(\lambda)$ of leaves. They are the spectral variables of the plate model that must be determined wavelength by wavelength. Because leaves cannot be regarded as compact layers, the structure parameter N representing leaf anatomy must also be determined. N changes from leaf to leaf and is assumed to be wavelength independent, but it cannot be directly measured. For this reason, the calibration was split into two steps that distinguish the assessment of N and the assessment of both k_{spe} and n .

1.4 Calculation of spectral indices

A number of spectral indices specifically designed to quantify the leaf chlorophyll and water and dry matter contents are applied in this study (Table 1). These are the optimal indices retrieved from studies in which a wide range of species, leaf structures, developmental stages, and spectral indices were tested (Le Maire *et al.*, 2004). Few of these indices, however, have been evaluated in arid ecosystems. Hence, we intend to examine the performance of these hyperspectral indices in arid ecosystems. Besides these indices, other wavelengths, the Simple Ratio ($SR=R_a/R_b$) and the Normalized ($ND=(R_a - R_b)/(R_a + R_b)$), were tested as well. The best spectral indices were determined through empirical models based on available data pools that were randomly divided into calibration and prediction sets: two-thirds of the data were used for calibration and one-third for validation.

1.5 Performance evaluation

To evaluate the ability of the inversed PROSPECT model and spectral indices to estimate the Chl, LMA, and EWT, we used two main statistical parameters,

Table 1 Spectral indices tested for Chl, EWT and LMA

Spectral index	Formula	Property estimated	Reference
ND (750, 705)	$(R_{750}-R_{705})/(R_{750}+R_{705})$	Chl	Gamon and Surfus (1999)
mND (750, 705)	$(R_{750}-R_{705})/(R_{750}+R_{705}-2R_{445})$	Chl	Sims and Gamon (2002)
SR (715, 705)	R_{715}/R_{705}	Chl	Vogelman <i>et al.</i> (1993)
SR (554, 667)	R_{554}/R_{667}	Chl	Smith (1995)
WI (970, 900)	R_{970}/R_{900}	EWT	Peñuelas (1994)
SR (1300, 1450)	R_{1300}/R_{1450}	EWT	Seelig (2008)
MDWI	$(R_{860}-R_{1240})/(R_{860}+R_{1240})$	EWT	Eitel (2006)
SR	R_a/R_b	All	This study
ND	$(R_a-R_b)/(R_a+R_b)$	All	This study

Note: R_a (R_b) is the reflectance at wavelength a (b); a and b range from 400 to 2,500 nm.

which were calculated as follows:

$$R^2 = 1 - \frac{\sum_{j=1}^n (y'_j - \bar{y})^2}{\sum_{j=1}^n (y_j - \bar{y})^2}, \quad (3)$$

$$RMSE = \sqrt{\frac{\sum_{j=1}^n (y'_j - y_j)^2}{n}}. \quad (4)$$

Where R^2 is the coefficient of determination, y' the estimated value, y the independent reference measurement, and root mean square error (RMSE) the absolute error in estimation.

2 Results

2.1 Polymorphic leaves and vertical profiles

Among tree species in arid lands, *P. euphratica* is known for its unusual leaves, which are lanceolate at the flushing stage, dentate broad-ovate at the growing stage, and broad-ovate when mature (Fig. 2). The lanceolate leaves grow mainly on the lower shoots of *P. euphratica* canopies, while the dentate broad-ovate leaves become more abundant with canopy height increases, and the broad-ovate leaves grow mainly in the middle parts of canopies (Fig. 3a). In the bottom layer of canopies (< 2 m height), the lanceolate leaves dominate and represent over 70% of the leaves. The remaining percentage of leaves in the bottom canopy consists largely of broad-ovate leaves, and dentate broad-ovate leaves appear only occasionally in the

bottom layer. In the middle layers, the broad-ovate leaves are prevalent, and the lanceolate leaves disappear rapidly with height increases and become rare at heights of > 2 m. Dentate broad-ovate leaves represent about 20% of the leaves in the middle layer and displays an increasing percentage as height increases. In the upper layers (> 6 m), dentate broad-ovate leaves are more abundant than broad-ovate leaves.

Not only the shape of *P. euphratica* leaves differs with heights, but also the biochemical constituents

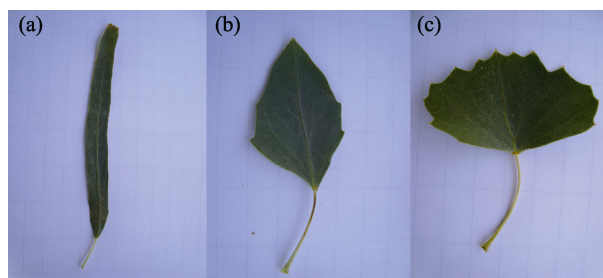


Fig. 2 Three shapes of *P. euphratica* leaves. (a) Lanceolate leaf; (b) Dentate broad-ovate leaf; (c) Broad-ovate leaf.

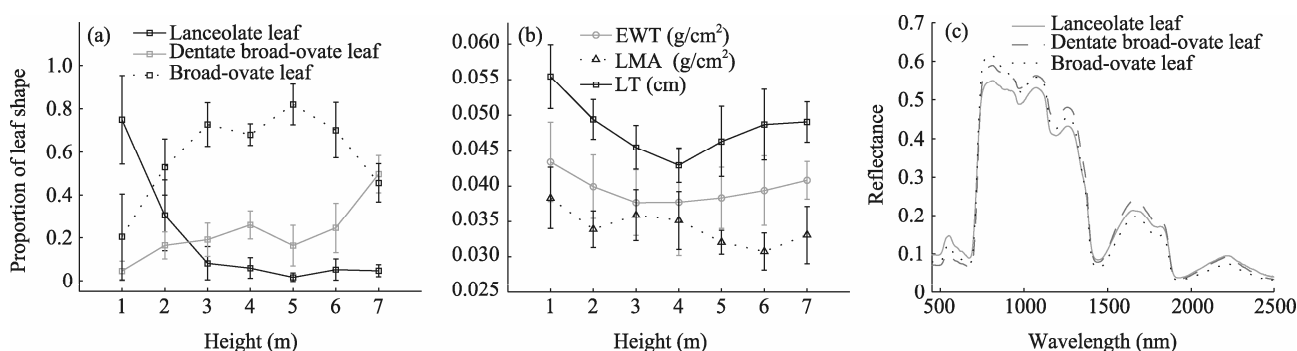


Fig. 3 Distribution of different types of *P. euphratica* leaves as a function of canopy height (distance from ground) and reflectance spectral variations of the different types of leaves.

change along the vertical profile of the canopy (Fig. 3b). EWT and leaf thickness (LT) share a similar trend. They both have the minimum values in the middle of the canopy, while LMA has the maximum value at 1-cm height.

Distinctive spectral characteristics were obtained for leaves with different shapes within the same canopy (Fig. 3c). Lanceolate leaves had the highest reflectance in the visible domain but low reflectance in the near-infrared domain of up to 1,400 nm. Lanceolate leaves had intermediate reflectance values (greater than dentate broad-ovate leaves but less than broad-ovate leaves) within the domain of 1,500 to 1,800 nm and had the highest values with wavelengths longer than 2,000 nm. The dentate broad-ovate leaves had the lowest reflectance values with wavelengths longer than 1,400 nm but had the highest values within the near-infrared domain. The broad-ovate leaves had the lowest reflectance values overall but had high reflectance values within the long wavelength domain ($> 1,400$ nm). Although the three spectra followed the same general pattern, some intersections between spectra occurred, especially in water absorption bands (Fig. 3c).

Biochemical properties also differed among the

three kinds of *P. euphratica* leaves. A plot of Chl on height produced a nearly parabola-shaped curve, in which the broad-ovate leaves that dominate the middle layer have higher Chl than the lanceolate or the dentate broad-ovate leaves. In the plot of Chl on canopy height, the Chl reached $92.6 \mu\text{g}/\text{cm}^2$ at the peak of the parabola-shaped curve and was 69.1 and $68.3 \mu\text{g}/\text{cm}^2$ at the curve endpoints. The maximum difference in the Chl of different leaf types was as high as 35.6%. However, the values of LMA, EWT, and LT were all lower in broad-ovate leaves of the middle canopy than in lanceolate leaves of the bottom canopy or the dentate broad-ovate leaves of the upper canopy. The LMA values ranged from 0.032 to $0.038 \text{ g}/\text{cm}^2$, and the EWT values ranged from 0.038 to $0.044 \text{ g}/\text{cm}^2$. The maximum difference was about 16% in both LMA and EWT values.

The results indicated that biochemical properties (such as Chl, EWT, and LMA) differ substantially among the three kinds of *P. euphratica* leaves and along the vertical axis of the *P. euphratica* canopy.

2.2 PROSPECT calibration and inversion

The PROSPECT model must be calibrated, especially with regard to the refractive index $n(\lambda)$, before it can

be inversed to estimate leaf biochemical properties. We applied the method of Feret *et al.* (2008) to calibrating $n(\lambda)$. The data used for calibration were randomly selected from the dataset and represented about 10% of the total data.

Because *P. euphratica* leaves have three main shapes, we applied two calibration strategies to the inversed PROSPECT model. In the first strategy, the model was calibrated once for all three types of leaves, and in the second strategy, the model was calibrated separately for each type of leaf. Figure 4 shows the calibrated refractive indices of both calibration strategies and the original refractive index that is the default in the PROSPECT-4. The calibrated refractive indices based on all three leaf types ('all calibration' in Fig. 4) were lower than the indices based on individual leaf types for most wavelengths, especially within the domain from 800 to 2,500 nm. Interestingly, all of the calibrated refractive index curves generally followed a similar pattern that differed from the default in the PROSPECT-4 model, especially in the wavelengths longer than 800 nm. The four calibrated refractive index curves were very similar at wavelengths of up to 750 nm and generally similar at wavelengths greater than 750 nm. While the calibrated refractive index for lanceolate leaves had the highest values among the four in the domain from 750 to 2,500 nm, the calibrated refractive index based on all types of leaves had the lowest values for the wavelengths longer than 1,400 nm, although it had higher values than the index for dentate broad-ovate leaves within the domain from 750 to 1,400 nm. Generally, the calibrated refractive indices were larger for lanceolate leaves and broad-ovate leaves than for all leaves ('all calibration' in Fig. 4) for the wavelengths of >750 nm, whereas the calibrated refractive indices for the dentate broad-ovate leaves were generally low.

The calibrated PROSPECT model can be tuned very punctually. The reflectance residuals are much lower (residual<0.02) in all wavelength domains if based on the calibrated model rather than on the default PROSPECT, thus the calibrated PROSPECT model can be used to accurately simulate the calibrated refractive index and the reflectance for the three different kinds of *P. euphratica* leaves.

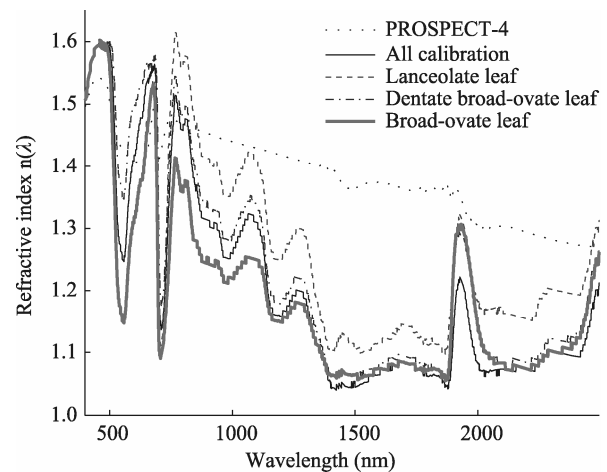


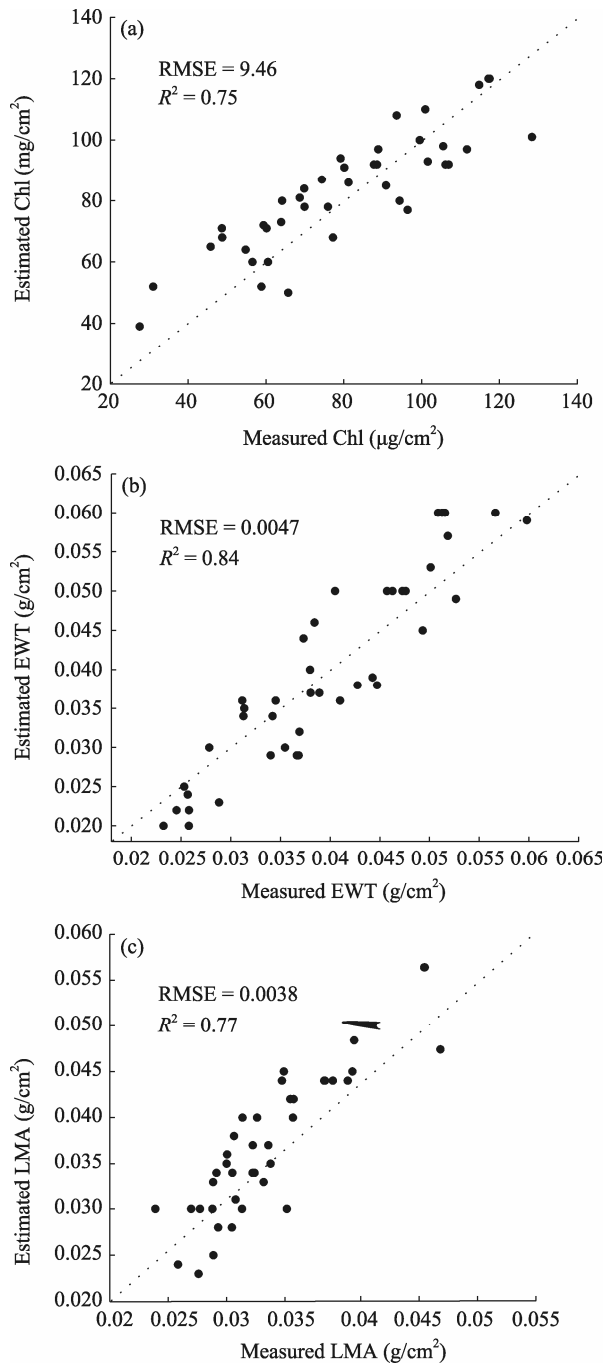
Fig. 4 Refractive index computed from the calibrated PROSPECT-4 model and the refractive index in the original PROSPECT-4 model.

The PROSPECT model with different calibrations was then inversed to retrieve leaf biochemical properties. The results of the inversions in terms of RMSE and R^2 are summarized in Table 2. The inversion model performed substantially better when the reflective index was calibrated individually for the three different leaf shapes rather than collectively for all three leaf shapes. The improvement was especially noteworthy for Chl, for which the RMSE decreased from 19.55 (based on calibration with all leaves) to 9.46 $\mu\text{g}/\text{cm}^2$ (based on calibration with three kinds of leaves); this was associated with an increase in the R^2 from 0.41 to 0.75. Although the inversed PROSPECT model with calibration for all leaves generally provided satisfactory results for estimating EWT ($R^2 = 0.64$), the inversed model performed better if calibrated for different leaf shapes, as indicated by the RMSE and R^2 values (Table 2). The same was true with the LMA estimation, in which the R^2 was increased from 0.62 to 0.77 and RMSE was reduced from 0.0065 to 0.0038 g/cm^2 when the inversed model was calibrated for different leaf shapes rather than for all leaf shapes. For all three biochemical properties, the inversed PROSPECT model calibrated for each leaf shape provided R^2 values >0.75 with significance at $P < 0.001$.

Figure 5 shows scatter plots of the measured biochemical properties versus the estimated properties as determined by the inversed PROSPECT model calibrated for different types of leaves.

Table 2 Validation of Chl, EWT and LMA estimated using the inversed PROSPECT model with two calibration methods

Property	Calibration method	RMSE	R^2	P
Chl	For all leaves	19.55	0.41	<0.001
	For three types of leaves	9.46	0.75	<0.001
EWT	For all leaves	0.0085	0.64	<0.001
	For three types of leaves	0.0047	0.84	<0.001
LMA	For all leaves	0.0065	0.62	<0.001
	For three types of leaves	0.0038	0.77	<0.001

**Fig. 5** Plots of estimated vs. measured Chl, EWT and LMA (the estimations were carried out with the calibrated PROSPECT-4 model).

2.3 Indices

Various hyperspectral indices reported from previous studies were examined for their performance on *P. euphratica*. In addition, we designed the simple counterpart (SR) and normalized indices (ND) types of indices and screened for all combinations of wavelengths at 1-nm intervals to identify the best indices. The results are presented in Table 3.

Table 3 Comparison of spectral indices from previous studies and new indices (indicated by bold font) identified in this study for estimating Chl, EWT and LMA

Property	Spectral index	RMSE	R^2	P
Chl	ND (750,705)	17.18	0.49	<0.001
	mND (750,705)	17.74	0.46	<0.001
	SR (715,705)	18.62	0.40	<0.001
	SR (554,667)	18.62	0.40	<0.001
	SR (750,705)	16.80	0.52	<0.001
EWT	WI (970,900)	0.0082	0.27	<0.001
	SR (1300,1450)	0.0083	0.25	0.001
	MDWI	0.0076	0.37	<0.001
	SR(1234,1309)	0.0049	0.74	<0.001
	ND (1234,1309)	0.0049	0.74	<0.001
LMA	SR (910,1075)	0.0046	0.51	<0.001
	ND (910,1075)	0.0046	0.51	<0.001

For Chl estimation, the previously reported indices performed poorly in the RMSE values ranged from 17.18 to 18.62 $\mu\text{g}/\text{cm}^2$ and R^2 values ranged from 0.49 to 0.40; these statistical parameters were far inferior to those resulting from estimations using the inversed PROSPECT model calibrated for the different leaf shapes. The lowest RMSE value and highest R^2 value for estimating Chl of *P. euphratica* leaves were obtained with the hyperspectral indices SR (750, 705) and ND (750, 705), which were identified in the current study. The determination of the waveband parameters (λ_1 and λ_2) of the SR and ND indices was performed by examining all possible combinations of wavelengths (λ_1 and λ_2) from 400–2,500 nm. For each combination, the index values were calculated for each spectrum of the dataset. An exponential regression was fitted between the index values and the leaf parameters (Chl, EWT and LMA). The RMSE and the coefficient of determination (R^2) are commonly used to compare the indices with different wavebands, and they were also used in this study. For a given index, the best combination of wavelengths should have the lowest RMSE and the highest R^2 .

The previously reported indices also performed poorly for EWT estimation. None of the three representative wave indices reported had an R^2 value larger than 0.40. The R^2 and RMSE values were greatly improved, however, with the hyperspectral indices SR (1234, 1309) and ND (1234, 1309), which were identified in the current study.

Because no hyperspectral index has been commonly applied for LMA estimation, we only used the best indices that were identified in this study. The results were encouraging in that both SR (910, 1075) and ND (910, 1075) had an R^2 of 0.51 and an RMSE of 0.0046 g/cm² when estimating LMA.

The previously reported indices were also tested in this study, in which the index of SR1300/1450 is the best one. However, it was found that the index of SR1234/1309 performed better than that of SR1300/1450 for estimating EWT, Chl or LMA based on R^2 values.

3 Discussion and conclusion

Researchers have previously attempted to estimate leaf biochemical properties by hyperspectra (Maccioni *et al.*, 2001; Strachan *et al.*, 2002; Pablo *et al.*, 2004), and the inversed PROSPECT model has been widely used to estimate leaf biochemical properties in various ecosystems (Baret and Fourty, 1997; Newnham and Burt, 2001). To the best of our knowledge, the current study is the first to apply the inversed PROSPECT model to estimating leaf biochemical properties of *P. euphratica*. This tree species dominating arid lands produces leaves with three different shapes within the same canopy, corresponding to different developmental stages. For the three leaf biochemical properties estimated (Chl, EWT, and LMA), we generally obtained RMSE and R^2 values similar to those obtained in other ecosystems. For instance, the RMSE values of 19.55 and 9.46 µg/cm² that we obtained for Chl using the inversed PROSPECT model with two different calibration strategies are well within the range of 5.17 to 32.35 µg/cm² reported by Feret *et al.* (2008). Similarly, our result based on the inversion model calibrated for different leaf shapes is very similar to that obtained by Jacquemoud *et al.* (2000), who reported an RMSE of 9.1. With respect to R^2 values, our result (0.75 µg/cm²) on Chl estimation with the inversion

model is better than that of Jacquemoud *et al.* (2008) and similar to that of Newnham and Burt (2001).

For EWT, we obtained an RMSE of 0.0047 g/cm² based on the inversion model calibrated for different leaf shapes, a value that is also within the range of 0.0017 to 0.0057 g/cm² presented by Feret *et al.* (2008) but much larger than that reported by Baret and Fourty (1997) and Jacquemoud *et al.* (2000). Regarding R^2 values obtained estimation of EWT with the inversion model, our R^2 value of 0.84 is smaller than that of Newnham and Burt (2001) and Riaño *et al.* (2005), who obtained R^2 values > 0.90. However, our result is better than that of Colombo *et al.* (2007), who obtained an R^2 of 0.65.

The RMSE of 0.0038 g/cm² for estimations of LMA by the inversion model in this study is also within the range reported by Feret *et al.* (2008), but much larger than those of Baret and Fourty (1997) and Jacquemoud *et al.* (2000). In former studies, however, R^2 values for LMA estimation ranged from 0.009 to 0.65 (Jacquemoud *et al.*, 2000), all of which are smaller than our R^2 value of 0.77. It follows that the results we obtained are comparable to those of other studies, indicating the feasibility of applying the inversed PROSPECT model to estimating leaf biochemical properties in arid ecosystems.

We found, however, the results obtained using the inversed PROSPECT model calibrated only once for all leaves were inferior to those reported in other studies. For EWT and LMA, the results based on the inversed PROSPECT model calibrated only once for all leaves cannot cover ranges provided by Feret *et al.* (2008). The poor performance with single calibration in our study relative to other studies probably reflects the dramatic difference in morphology and anatomy of the three kinds of leaves produced by *P. euphratica*. This leaf polymorphism requires that each kind of leaf be calibrated for *P. euphratica*.

One of the peculiar properties of *P. euphratica* is that three differently shaped leaves grow right in the same *P. euphratica* canopy. The biochemical and spectral parameters of these leaves are significantly different, and some large errors of these parameters will be brought in if these leaves are not considered separately, which is one of the main results in this paper. Moreover, the contribution of broad-ovate leaves to the spectral and satellite RS values of canopy is

possibly high because broad-ovate leaves grow mainly in the upper part of canopy, but it needs to be further researched in the future.

To investigate the calibration problem further, we have carried out a residuals analysis for estimations of biochemical properties based on the inversed PROSPECT model calibrated only once for all three kinds of leaves. The residuals analysis for Chl revealed that the estimation for the leaves in the upper canopy (at 7-m height) produced a higher RMSE ($23.17 \mu\text{g}/\text{cm}^2$) than estimations for those in the middle and lower canopy. As indicated in the introduction, the upper canopy layer contains both dentate broad-ovate and broad-ovate leaves. The poor result in the upper canopy therefore supports the idea that calibrating all three kinds of leaves only once is ineffective. For the six sampled trees, the residuals of EWT and LMA estimated by the inversed PROSPECT model calibrated for all shaped leaves were all lower than 0.01.

According to groundwater levels measured from six monitoring wells near the sampled trees, the residuals of EWT increased with the increase of groundwater depth (unpublished data). This suggests that the inversed PROSPECT model performs poorly as drought increases in ecosystems. This finding is preliminary, however, and the relationship between the performance of the inversed model and drought requires further investigation.

Our results clearly indicated the importance of calibration for estimation of leaf biochemical properties using the inversed PROSPECT model. For canopies that contain different-shaped leaves, it is necessary to calibrate the inversion model for each leaf shape. In our study, for instance, the RMSE values for estimations of Chl, EWT and LMA from the model inversion were reduced by about 50% if the model was calibrated for different leaf shapes separately rather than for all leaves collectively. Calibration for different leaf shapes also substantially increased the R^2 values for estimation of Chl, EWT and LMA. The findings represent a challenge to the approach that is commonly used for simulating canopy-scale reflectance, which requires upscaling from leaf to canopy and which is usually based on a combination of a leaf-scale reflectance model (e.g. PROSPECT, Jacquemoud *et al.*, 1990) with a canopy structure description model (e.g.

SAIL, Verhoef, 1984), as in the most popular PROSAIL family models. To our knowledge, there is no such calibration strategy that calibrates the leaf-scale model with different shaped leaves. The current results therefore indicate that applying such models to canopy-scale reflectance simulation as well as to further inversion applications in canopies containing leaves with different shapes is problematic. Recent attempts on estimating canopy-scale biochemical properties via the inversed PROSAIL model have been carried out in several studies (Zarco-Tejada *et al.*, 2004), in which the vertical changes of biophysical and biochemical properties as well as specific requirements on calibration strategies associating with different leaf shapes have not been explicitly treated. This casts doubt on the application of such inversed models to deriving canopy-scale biochemical properties for canopies with obvious vertical changes in leaf type. This problem should be addressed in future canopy-scale reflectance modeling before such models can be applied inversely to estimating biochemical properties.

Remote sensing indices represent an alternative approach for estimating leaf biochemical properties. They are becoming more popular than the inversion model approach because of their easy application. Numerous hyperspectral indices (Table 1) have been reported to be closely related to leaf biochemical properties like Chl and EWT. These previously reported indices, however, generally performed poorly for *P. euphratica*. This is because these indices were developed under completely different environments, and the empirical approach is widely acknowledged for its limitations in spatio-temporal applications. The current study identified the best hyperspectral indices for estimating Chl and EWT in arid ecosystems. Both SR (750, 705) and SR (1234, 1309) or ND (1234, 1309) provided satisfactory estimations of Chl and EWT (Table 3). While the performance of the newly identified hyperspectral index SR (750, 705) was not much superior to other reported indices in estimating Chl, SR (1234, 1309) or its equivalent ND (1234, 1309) were superior in estimating EWT for arid ecosystems, in terms of both R^2 and RMSE. As no hyperspectral index has been previously reported for LMA estimation, the indices reported here are the first ones, and both SR (910, 1075) and ND (910, 1075) provided reasonable estimation of LMA in arid lands. Because

they are easy to use, we foresee the wide application of the indices identified in this study to estimating leaf biochemical properties in arid ecosystems.

As already noticed, the selected wavelengths are similar for ND or SR, and the R^2 and RMSE performances are comparable. The normalized indices were introduced to avoid the effects of differences in constant background terms for normalized reflectance-based indices (e.g. different atmospheric conditions or soil moisture in the case of canopy measurements). Here, at the leaf level, no improvement for any biochemical parameter estimation is observed since all reflectance spectra are measured with a dark background. When calibrated and used with canopy level data, an improvement of the ND indices (compared to their SR indices) may be expected.

In conclusion, both the inversed PROSPECT model and hyperspectral indices were applied to estimating biochemical properties of *P. euphratica* leaves. *P. euphratica* is a dominant species in arid lands and is known for its vertical variations in both leaf morphologic and biochemical properties. The results indicated that the inversed PROSPECT model can be used to satisfactorily estimate leaf biochemical properties if calibrations have been carried out for each of the three types of *P. euphratica* leaves, but that model perform-

ance is generally poorer than reported in other ecosystems if the calibration is performed only once for all types of leaves. This finding suggested that for canopies with clear vertical variations, researches should be cautious in applying inversed models to estimating canopy-scale biochemical properties when the calibration has not yet recognized the leaf variation within the canopy.

In addition, previously reported hyperspectral indices generally performed poorly in the arid ecosystem of the current study. The hyperspectral indices identified in this paper, SR (750, 705) for Chl, SR (1234, 1309) or its equivalent ND (1234, 1309) for EWT, and SR (910, 1075) or ND (910, 1075) for LMA, can all provide reasonable estimation to the biochemical properties of leaves adapted to arid environments. These hyperspectral indices should be widely applied because they are both robust and easy to use.

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