

## AN INVERSION APPROACH FOR BIOCHEMICAL PARAMETERS OF VEGETATION BASED ON THE PROSPECT-5 MODEL

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### ABSTRACT:

Accurate inversion of vegetation biochemicals using the PROSPECT model mostly depends on a proper inversion approach, including a suitable optimizing algorithm, appropriate dependent variables, and different properties from spectra of reflectance (R) and transmittance (T). In this paper, we propose a special inversion method using PROSPECT-5 and then explore its effectiveness in inverting chlorophyll, carotenoids, equivalent water thickness, and dry matter per area data from the ANGERS database. The inversion strategy includes (i) an optimal algorithm with constrained bounds (fminsearchbnd) to replace the common function fminsearch, (ii) and four parameters are considered together and separately as dependent variables of models, (iii) Using properties from the spectra of R, T and combined R&T to invert the above four biochemical parameters. The results show that fminsearchbnd can improve the model's  $R^2$  based on a field-measured database. Moreover, using the entire set of parameters together as the model inputs is more effective than using single parameters separately. T spectra are favoured for all parameter inversions in the model database while being inapplicable in the ANGERS database. These findings provide an appropriate inversion strategy for the PROSPECT-5 model in vegetation biochemical parameters analysis and suggest further research to develop an accurate inversion process for vegetation based on various physical models.

### 1. INTRODUCTION

Vegetation is a significant aspect of the earth's ecosystems that strongly impact humans' daily lives. Dense and green vegetation on land offers a natural source of oxygen, a comfortable living environment, and absorption of greenhouse gases, such as CO<sub>2</sub> (Krupa, S.V. and R.N. Kickert., 1989; Kimball, B.A., et al., 1992). The situation of vegetation is an important comprehensive index to measure the ecological environment (SUN H Y, LI B., 1998). Timely and accurately grasp the situation of vegetation growth has important practical significance for the sustainable development of city and natural environment. The monitoring information of vegetation situation has been mainly achieved by combination of field measurements, which plays excellent performance in terms of high accuracy and low error in a small area. But the monitoring of vegetation growth often involves a wide range, many contents and complex topography, it is easily influenced by subjectivity of human and heterogeneity of ground spatial (Wang Qiao., 2021). These impacts lead to the requirement of accuracy of vegetation monitoring information are difficult to meet in a large area. Remote sensing monitoring technology can be used as wide coverage and continuity of time and space (XIONG J N, PENG C, CHENG W M, et al., 2018; LI C X, GONG J, DENG F, et al., 2019). To a certain extent, these advantages can make up for the shortcomings of field measurement methods in large-scale regional monitoring (LI C X, DENG F, ZHANG J H, et al., 2019). In recent years, the research of monitoring information of vegetation situation based on remote sensing technology has been drawn widely attention by scholars of remote sensing. Data on vegetation research primarily focuses on passive remote sensing technology, which

is based on the different spectral characteristics of reflectance (R) and transmittance (T) related to different environmental stresses (Adam, E., O. Mutanga, and D. Rugege., 2010; Semeniv, O.V., 2016). These differences can be utilized to analyse the growth status of vegetation. In this paper, we employ the PROSPECT-5 model for biochemical parameter analysis using a special inversion strategy.

Several parameters affect the growth status of vegetation and are detectable as differences in R and T spectra (Semeniv, O.V., 2016). These parameters include biochemical parameters, such as chlorophyll (Cab), carotenoids (Car), and water, and structural parameters, such as leaf structure index (N) and leaf area (Yansong, B., L. Liangyun, and W. Jihua., 2008). Accurate inversion of these parameters, especially biochemical parameters, plays an important role in vegetation analysis (Pu, R. and P. Gong., 2011). Researchers typically analyse the relationship between R and T spectra and biochemical parameters by using statistical methods and optimization algorithms (Adam, E., O. Mutanga, and D. Rugege., 2010; Okin, G.S., et al., 2018), however, although some satisfactory results have been obtained, the conclusions obtained in particular environments are inapplicable to new environments. Hence, studies to design a universal method for analysis of vegetation growth status are needed. In this regard, the leaf model PROSPECT proposed by Jacquemoud (Jacquemoud, S. and F. Baret, PROSPECT., 1990) is the most successful way to invert the biochemical parameters of vegetation.

The PROSPECT model is developed from the plate model (Richardson, A.J., et al., 1969) and is based on the interaction between solar radiation and the pigments or inner structure of

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leaves. One of the latest versions of this model is PROSPECT-5, which can simulate the R and T spectra of leaves using N, Cab, Car, equivalent water thickness (EWT), and dry matter per area (LMA) (Feret, J.B., et al., 2008; F  ret, J.B., et al., 2017; Sun, J., et al., 2018). By running this model in forward mode, a large synthetic spectral database encompassing the wavelengths of 400 to 2500 nm can be generated. The common inversion process of PROSPECT-5 requires R and T spectra as model inputs, but the spectra of R and T over wide wavelength bands are closely correlated with each other and are sensitive to certain parameters. Thus, an appropriate inversion strategy, such as analysing each parameter at a multi-stage process according to its sensitivity, is significant for the efficient inversion process. We designed a strategy to study the effect of different spectral properties derived from R and T on inversion results. With synthetic spectra or field measured data, the biochemical parameters of vegetation can be inverted using optimal algorithms, proper cost functions, and appropriate dependent variables. These conditions constitute an inversion strategy for biochemical parameters, which is important for the accurate analysis of vegetation growth status.

In this paper, an inversion strategy for the PROSPECT-5 model is designed as follows: (a) a derivative function of *fminsearch* called *fminsearchbnd* is used to study whether the constrained bounds are effective and sensitive to the inversion results; (b) four biochemical parameters (Cab, Car, EWT, and LMA) are inverted simultaneously, and the result is compared with separately inverting each parameter; and (c) spectra of R, T and R&T are separately selected as inverting parameters.

## 2. MATERIALS AND METHODS

### 2.1 Materials

The quantity and quality of analysis samples determine the accuracy and reliability of our experimental results. Data used in this paper are from two sources: ANGERS database and Modelled database.

#### 2.1.1 ANGERS database

Catalogue	ANGERS
Date	2003
Number of sample	276
Number of species	49
Spectrophotometer/ spectroradiometer	ASD FieldSpec
Spectral range	400 – 2450 nm
Spectral sampling	1.4 nm (350 – 1050 nm)
	2 nm (1000–2500 nm)
Solvent	Ethanol 95%
Method for pigments	Lichtenthaler (1987)

Table 1 summarizes the main characteristics of the ANGERS database including information of time, Number of sample, Number of species, Spectrophotometer/spectroradiometer, Spectral range, Spectral sampling and Solvent Method for pigments (Feret, J.B., et al., 2008).

Catalogue	degree	Measured value
Chlorophyll a (��g/cm <sup>2</sup> )	Min	0.4
	Max	76.8
	Mean	25.4
Chlorophyll b (��g/cm <sup>2</sup> )	Min	0.3
	Max	29.9
	Mean	8
Carotenoids (��g/cm <sup>2</sup> )	Min	0
	Max	25.3
	Mean	8.7
Water (cm)	Min	0.0044
	Max	0.0340
	Mean	0.0116
Dry matter (g/cm <sup>2</sup> )	Min	0.0017
	Max	0.0331
	Mean	0.0052

Table 2 summarizes the main measured value information of the types of biochemical constituents. The types include five types: chlorophyll a (Ca), chlorophyll b (Cb) and total carotenoid (Car) content, water depth (Cw or EWT for equivalent water thickness), and dry matter content (Cm or LMA for leaf mass per area) (Feret, J.B., et al., 2008).

One source is the ANGERS database, established in June 2003 in Angers, France (Feret, J.B., et al., 2008). This database includes 276 leaf samples representing a large variety of typical plant species. The data of transmittance spectra and leaf directional–hemispherical reflectance measured in the optical range (b2 nm step) with laboratory spectrophotometers or field spectroradiometers equipped with integrating spheres was used to making the datasets of ANGERS database. The types of biochemical constituents include five types: chlorophyll a (Ca), chlorophyll b (Cb) and total carotenoid (Car) content, water depth (Cw or EWT for equivalent water thickness), and dry matter content (Cm or LMA for leaf mass per area) (Feret, J.B., et al., 2008). In ANGERS, R and T spectra of leaves were measured using laboratory spectrophotometers or field spectroradiometers with a spectral interval of 1 nm. Table 1 and table 2 summarize the main characteristics of the ANGERS database.

#### 2.1.2 Modelled database

The other database is composed of spectra modelled using PROSPECT-5. Four biochemical parameters (Cab (chlorophyll a and chlorophyll b), total Car (carotenoid content), EWT (water depth) and LMA (dry matter content)) are selected to validate the inversion strategy employed in this paper, and their bounds are set using measured maximum and minimum values in the ANGERS database. We assume that parameter values follow a Gaussian distribution within the range of [Minx, Maxx] (x represents the biochemical parameters) then establish the database by generating different parameter sets.

## 2.2 Methods

The inversion strategy of using the PROSPECT-5 model to generate biochemical parameter sets is carried out with an optimizing algorithm called Nelder-Mead (N-M) method. The study evaluates whether simultaneously or separately inverting the four parameters (Cab (chlorophyll a and chlorophyll b), and total Car (carotenoid content), EWT (water depth), and LMA (dry matter content)) yields the most effective results. The spectral properties from R and T spectra are treated respectively. The N-M method with no limitation bounds is a commonly applied method for finding the minimum or maximum of nonlinear optimization problems, the derivatives of which may be unknown in n-dimensional space. This method is also called the downhill simplex method or the amoeba method (Nelder, J.A. and R. Mead., 1965), proposed by Nelder and Mead (Press, W.H., 1992) as a development of the method of Spendley et al. (Spendley, W., G.R. Hext, and F.R. Himsworth., 1962).

The N-M method uses a polyhedron (having  $n+1$  vertexes) to approach the optimal point by updating the worst vertex  $x_{n+1}$  with a new best point. Assuming that  $x_1, \dots, x_{n+1}$  are the vertexes of a polyhedron and satisfy, and the worst vertex is the maximum point of a function  $f(x)$ , then

$$f(x_1) \leq f(x_2) \leq \dots \leq f(x_{n+1}) \quad x \in R^n \quad (1)$$

There are four updated settings for this method: reflection, expansion, external contraction, and internal contraction. If these four processes cannot reach an optimal solution, the search intervals will be successively contracted to find the optimal point. This optimization process can be resolved depending on several coefficients that control its search speed and direction (Kolda, T.G., R.M. Lewis, and V. Torczon., 2003; Lewis, R.M., A. Shepherd, and V. Torczon., 2005; Yu, W.C., 1979). This method is carried out using Matlab 2014b and, based on a function called `fminsearch` from which a derived function with constrained bounds, `fminsearchbnd` (Luersen, M.A. and R.L. Riche., 2004), is then applied to estimate the

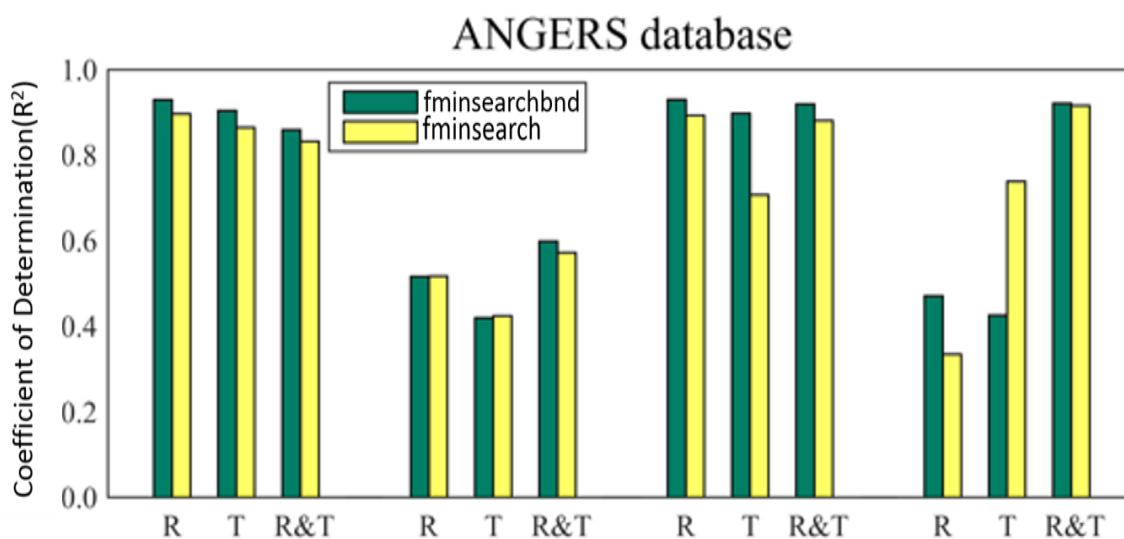
sensitivity and effectiveness of constrained bounds on the inversion results of the PROSPECT-5 model.

## 3. RESULTS AND DISCUSSION

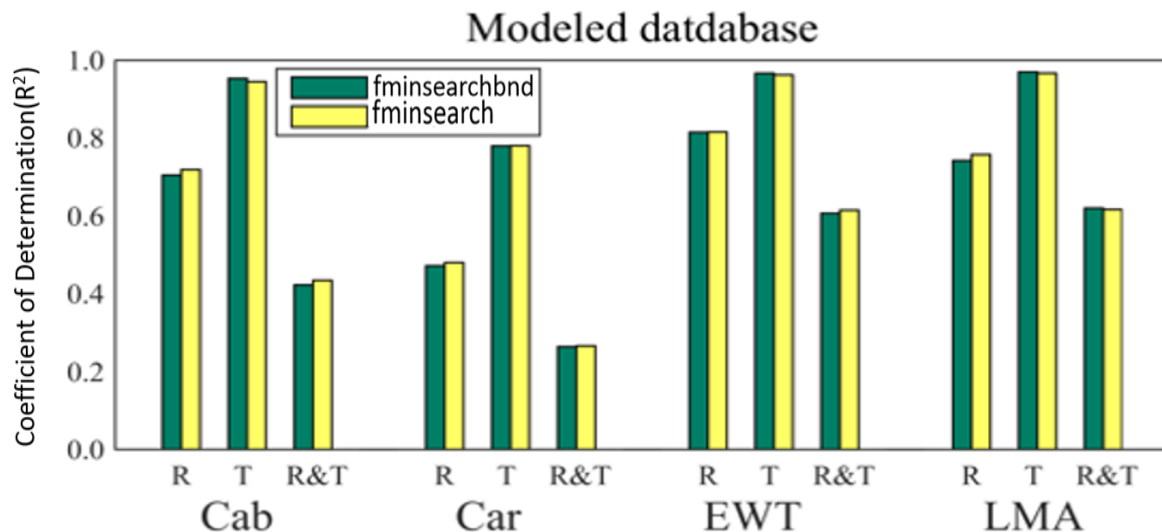
Different inversion strategies yield different inversion results, and sometimes the differences between these results are not close. Therefore, choosing an appropriate inversion strategy will help improve the reliability of the experimental results. The optimal algorithm, named `fminsearchbnd`, improves inversion results and the calculation efficiency of measured field data. Using biochemical parameters (Cab(chlorophyll a and chlorophyll b), and total Car (carotenoid content), EWT (water depth), and LMA (dry matter content)) as separate dependent inputs for the inversion process is compared with inverting all of the parameters simultaneously, which is the main inversion strategy for biochemistry parameters in this paper. Different spectra, including R and T, containing abundant, diverse but relevant information, have been correlated to all of the parameters (Cab(chlorophyll a and chlorophyll b), and total Car (carotenoid content), EWT (water depth), and LMA (dry matter content)) to estimate sensitivity and effectiveness for special parameters inversion. The results of this inversion strategy are described below. The databases are from ANGERS and the synthesized values generated using the PROSPECT-5 model.

### 3.1 Parameters inversion using the N-M method with bound constraints

In general, the  $R^2$  of simultaneously inverting four parameters with the N-M method is greater than 0.6, except in the case of Car contents in the ANGERS database. Even so, by using the spectra of R+T, the  $R^2$  of Car can be increased to 0.5988 (Figure. 1). Compared with the function without bound constraints, the `fminsearchbnd` function generally improves inversion results based on the ANGERS database except for LMA using T spectra, in which case the method of `fminsearch` yields a  $R^2$  of  $> 0.9$ , which is considerably higher than that obtained using `fminsearchbnd`.



**Figure 1.** Values of coefficient of determination ( $R^2$ ) using the N-M method to invert biochemical parameters based on the spectra of reflectance (R), transmittance (T) and both (R&T). The data are from ANGERS database.



**Figure 2.** Values of coefficient of determination ( $R^2$ ) using the N-M method to invert biochemical parameters based on the spectra of reflectance (R), transmittance (T) and both (R&T). The data are from modelled database.

In Figure. 1, although the model  $R^2$  for results based on the T spectra is lower than that using R spectra, improvement of the inversion results resulted from adding R+T spectra as the input of the cost function of the inversion model. In contrast to the ANGERS database, use of the modelled database does not considerably improve the inversion results when the fminsearchbnd algorithm is applied; however, for the modelled database, the T spectra yield the highest  $R^2$  for all four parameters, regardless of the algorithm used (Figure. 2). The T spectra are generated after light penetrates into plant leaves or canopy, reacting with many pigments, such as Car and Cab, within their inner structure. This finding may explain why using T spectra for model inversion yields better results in the modelled database than in the ANGERS database.

In Figure. 1 and Figure. 2, the N-M method with bound constraints can be considered the prior choice for biochemical parameter inversion. By taking the relationship between each parameter and spectral characteristic into account, variables of R, T, or R+T spectra can enhance the inversion ability of the physical model. According to the distribution range of the parameters, algorithms with bound constraints can reduce unnecessary calculations in the optimization process and shorten the search time. Different parameters are related or sensitive to some spectral variables; therefore, selecting the proper spectral characteristics and constrained conditions for the inversion model can improve the results. Thus, the inversion strategy described in this paper can provide effective guidance for biochemical parameter inversion based on the physical model. Certainly, there are many outstanding algorithms for optimize the cost function of PROSPECT-5, varying from common statistic regression to numerous intelligent algorithms. A worthy future work would be to find the proper ones for inversion of specific parameters, highlighting their advantages and then applying them to the inversion of biochemical parameters in practice.

### 3.2 Separate inversion of parameters

The parameters are sometimes correlated with each other, especially those that have close relationships in both the visible or near infrared bands. Selecting a single biochemical parameter as the input of the cost function, avoiding the mixed sensitive bands range, affects the inversion results. In this study, we employ an inversion strategy using fminsearchbnd to separately invert four biochemicals based on spectra of R, T, and R&T. The resulting  $R^2$  values are listed in Table 3. Unsatisfactorily, this inversion strategy does not improve the  $R^2$  considerably and yields poorer results in most cases, especially when using T spectra for all parameters. For the Cab,  $R^2$  is  $>0.9$  when all four parameters are inverted simultaneously based on R spectra, but when the input of the cost function of the inversion model is Cab only,  $R^2$  is  $<0.9$  and even drops to  $<0.3$  when using T spectra. Moreover, the availability of the T spectra for model inversion deteriorates gradually, and the R+T spectra become less advantageous for inversion of the parameters, especially for Cab and EWT in the ANGERS database. This result is inconsistent with that generated using the modelled database (Figure. 2).

The inversion strategy in this study significantly improves the inversion model results for the biochemical parameters, especially when using the optimal algorithm with bound constraints to replace the fminsearch function. However, improvements in parameter inversion resulting from single-parameter inputs to the cost function are suboptimum. In contrast, by combining the four biochemistry parameters together as the dependent variables of an inversion model, the results are improved. In fact, there are many factors that may affect the results as single-parameter inputs, such as vegetation type, and conditions of spectra collection, such as sites, and years. Such factors can be the subject of future work. Wide range spectral bands (e.g., 400-2450 nm for the ANGERS database) contain many useful information, but also possibly being redundant and noisy for parameters inversion. For this reason, sensitive band selection before generating models is another necessary and important inversion strategy.

Catalogue	The types of variable					
Variable	All variables used for inversion			Single variable used for inversion		
Spectra	R	T	R&T	R	T	R&T
<b>Cab</b>	0.9299	0.9044	0.8596	0.8696	0.2301	0.7167
<b>Car</b>	0.5163	0.4199	0.5988	0.4704	0.1572	0.5116
<b>EWT</b>	0.9303	0.8980	0.9196	0.7847	0.1660	0.5768
<b>LMA</b>	0.4711	0.4258	0.9214	0.5437	0.1092	0.3430

**Table 3.** Comparison of  $R^2$  values by using all variables and single variables for the inversion model based on the spectra of R, T and R&T. The database is ANGERS and optimal algorithm for cost function is fminsearchbnd.

#### 4. CONCLUSIONS

The PROSPECT model has been applied in many fields and has mostly achieved satisfactory results. In this paper, we employ the PROSPECT-5 model for biochemical parameter analysis using a special inversion strategy. The results show that a good inversion strategy is as significant as the classical physical model for vegetation analysis, and we can select a proper and effective inversion strategy for different goals. By choosing the optimal algorithm and proper input variables of the cost function for the inversion model, satisfactory results can be achieved. Although the results obtained after separating parameters into inversion function inputs are not ideal compared with using all parameters simultaneously, the proposed inversion strategy in this study may represent a valuable attempt to carry out vegetation analysis based on the PROSPECT-5 model.

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