Postprint of Hyperspectral Estimation of Rice Pigment Content Based on Band Depth Analysis and BP Neural Network

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Abstract

Based on a rice field nitrogen fertilizer level experiment, this study established a hyperspectral estimation model for rice pigment content using univariate linear and nonlinear regression methods. Analysis of the estimation capability of various vegetation indices for pigment content revealed that vegetation indices suffer from saturation problems at high pigment content levels. To address this, Band Depth Analysis (BDA) was combined with a BP neural network to improve the accuracy of hyperspectral estimation of rice leaf pigment content. Based on continuum removal processed rice canopy hyperspectral data (400–750 nm), four band indices were selected: Band Depth (BD), Band Depth Ratio (BDR), Normalized Band Depth Index (NBDI), and Band Depth Normalized Area Index (BNA). Principal Component Analysis (PCA) was then performed for dimensionality reduction, followed by hyperspectral inversion of rice leaf pigment content using a Back Propagation (BP) neural network method, to explore the possibility and effectiveness of combining BDA with BP neural networks in solving the vegetation index saturation problem. The results demonstrated that Band Depth Analysis highlighted differences in spectral absorption features, extracted more potential information, and enhanced the differentiation of spectral curves. The estimation model combining BD with BP achieved the highest accuracy for estimating carotenoid content in rice leaves (R^2=0.61, RMSEP=0.128 $mg \cdot g^{-1}$), while the model combining BNA with BP achieved the highest accuracy for estimating chlorophyll content (R^2=0.73, RMSEP=0.343 $mg \cdot g^{-1}$). Comparative analysis of the accuracy between BDA-BP combined models and the optimal regression models based on vegetation indices revealed that the BP neural network model established through Band Depth Analysis could effectively mitigate the saturation problem and improve the estimation accuracy of rice leaf pigment content.

Full Text

Preamble

Hyperspectral Estimation of Rice Pigment Content Based on Band Depth Analysis and BP Neural Network

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Abstract: Conventional vegetation indices exhibit reduced sensitivity to pigment content variation when pigment levels are high, leading to low estimation accuracy. To improve the accuracy of rice carotenoid and chlorophyll content estimation using canopy reflectance across all growth stages, this study explores the feasibility and effectiveness of combining band depth analysis (BDA) with back propagation (BP) neural networks to address vegetation index saturation. Using canopy hyperspectral data (400–750 nm) processed via continuum removal, four band indices—band depth (BD), band depth ratio (BDR), normalized band depth index (NBDI), and band depth normalized to band area (BNA)—were calculated. Principal component analysis (PCA) was employed for dimensionality reduction, and the resulting components were used as input variables for BP neural network models to invert rice leaf pigment content. Field experiments were conducted in Meichuan Town, Hubei Province, with eight nitrogen fertilization treatments (0, 45, 82.5, 127.5, 165, 210, 247.5, and 292.5 $kg \cdot hm^{-2}$) to generate varying vegetation and pigment levels. Linear and nonlinear regression models quantitatively analyzed relationships between vegetation indices and measured pigment content, with coefficient of determination (R^2) and root mean square error (RMSE) used for model evaluation. Results demonstrate that BDA highlighted differences in spectral absorption characteristics, revealing more potential information and enhancing spectral differentiation. The BD-BP model achieved the highest estimation accuracy for leaf carotenoid content ($R^2 = 0.61$, RMSEP = 0.128 $mg \cdot g^{-1}$), while the BNA-BP model performed best for chlorophyll content ($R^2 = 0.73$, RMSEP = 0.343 $mg \cdot g^{-1}$). Compared with the optimal regression models based on vegetation indices, the BDA-BP neural network models effectively mitigated saturation problems and improved estimation precision for rice leaf pigment content.

Keywords: Hyperspectral; Rice; Pigment; Vegetation index; Band depth analysis; Principal component analysis; Back propagation neural network

Introduction

Pigment content serves as a crucial indicator of crop physiological status, with its variation providing an effective means to assess photosynthetic capacity and primary productivity. Real-time, rapid acquisition of pigment content information has become an essential method for monitoring rice (*Oryza sativa*) growth, development, and yield. Traditional laboratory physicochemical analysis of crop leaf pigment content is time-consuming, labor-intensive, and destructive. In recent years, hyperspectral technology has offered an effective approach for rapid, efficient, and non-destructive detection of crop leaf pigment content, owing to its strong band continuity, high spectral resolution, and rich spectral information [1-2]. Consequently, research on quantitative estimation of crop pigment content using hyperspectral technology holds significant practical importance.

Within the visible range, vegetation canopy reflectance spectra are primarily influenced by leaf pigment content, whereas in the near-infrared range, leaf structure, biomass, protein, and water content play dominant roles. Numerous studies have demonstrated that pigment content can be estimated from canopy reflectance spectra [3]. Crop leaf pigments mainly comprise chlorophyll (chlorophyll *a* and *b*) and carotenoids (carotene and xanthophyll), with chlorophyll being the primary light-absorbing substance that directly affects light energy utilization in photosynthesis. Research indicates that chlorophyll *a* and *b* have absorption peaks at 665 nm and 643 nm, respectively, while carotenoid absorption peaks overlap with those of chlorophyll, making independent estimation of different pigments challenging. Literature reports show that multivariate statistical regression models established between remote sensing bands or vegetation indices and biochemical component contents can accurately estimate plant leaf biochemical composition. Wang et al. [2] developed normalized pigment indices for chlorophyll and carotenoids through pairwise combinations of all spectral bands, while Sims et al. [4] proposed new spectral indices for leaf pigment prediction. However, selected characteristic spectra and parameters vary significantly across different crops, experiments, and leaf structures. The most prominent issue is that conventional vegetation indices tend to saturate at high leaf pigment levels, substantially reducing estimation accuracy [5]. Lichtenthaler et al. [6] noted that NDVI is insensitive to high chlorophyll concentrations because its high sensitivity to chlorophyll absorption bands causes leaf light absorption to reach saturation at relatively low chlorophyll content.

To address this issue, Gitelson et al. [7-8] proposed that reflectance ratio vegetation indices at the red edge position (700 nm) are more sensitive to chlorophyll absorption characteristics. However, when leaf chlorophyll content changes, the corresponding absorption bands, red edge position, and red edge area also shift [9]. Continuum removal can correct band-dependent shifts in reflectance extrema, adjusting band peaks to their true positions [10]. Building upon this, band depth analysis of continuum-removed spectra enhances absorption features and reduces irrelevant information redundancy [11]. Mutanga et al. [12] applied band depth analysis to grass canopy spectra under controlled laboratory

conditions, combining it with stepwise multiple linear regression to estimate aboveground biomass. Kokaly et al. [13] successfully estimated biochemical content in dry leaves using band depth analysis, while Chen et al. [14] combined band depth analysis with PLS to estimate aboveground biomass in high-coverage grasslands.

Current quantitative analysis of vegetation canopy spectra often employs linear methods such as stepwise multiple regression and PLS. However, due to numerous influencing factors including weather, crop variety, soil background, and experimental conditions, the relationship between canopy spectra and plant leaf component content is nonlinear, which existing methods struggle to fit. Artificial neural networks have been widely applied due to their strong nonlinear processing, self-organizing adjustment, and adaptive learning capabilities. This study aims to improve the accuracy of canopy spectral estimation of rice carotenoid and chlorophyll content throughout the entire growth period by employing band depth analysis (BDA) to calculate band depth indices, followed by principal component analysis (PCA) for dimensionality reduction, to establish BP neural network models for predicting rice leaf pigment content and explore the potential and effectiveness of combining BDA with BP neural networks to solve vegetation index saturation problems.

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1 Materials and Methods

1.1 Experimental Materials

The field experiment was located in Meichuan Town, Wuxue City, Hubei Province (30°06 N, 115°35 E). The soil type was paddy soil with a pH of 5.70 in the 0–20 cm tillage layer, organic matter content of 37.35 $g \cdot kg^{-1}$, total nitrogen of 1.60 $g \cdot kg^{-1}$, available phosphorus of 5.83 $mg \cdot kg^{-1}$, and available potassium of 91.67 $mg \cdot kg^{-1}$. The rice cultivar was 'Shenliangyou 5814', a hybrid indica rice with a growth period of approximately 138 days and moderate plant architecture with erect leaves.

1.2 Experimental Design and Methods

The experimental field comprised 24 plots with eight nitrogen fertilization treatments: 0, 45, 82.5, 127.5, 165, 210, 247.5, and 292.5 $kg \cdot hm^{-2}$, designated as N0, N3, N5.5, N8.5, N11, N14, N16.5, and N19.5, respectively. Each treatment was replicated three times in a randomized block design, with each plot covering 20.0 m^2. Phosphorus and potassium fertilizers were applied at rates of 75 $kg \cdot hm^{-2}$ P_2O_5 and 75 $kg \cdot hm^{-2}$ K_2O. Nitrogen fertilizer was urea (46% N), phosphorus fertilizer was calcium superphosphate (12% P_2O_5), and potassium fertilizer was potassium chloride (60% K_2O), all applied as basal fertilizer. Planting density was 255,000 plants $\cdot hm^{-2}$. Seeds were sown on May 25, 2015, transplanted on June 28, and matured on October 9.

1.3 Measurements

1.3.1 Canopy Hyperspectral Reflectance Measurement Canopy spectral reflectance was measured during five key growth stages in 2015: tillering (July 10), jointing (July 27), booting (August 12), heading (August 27), and filling (September 12). On clear, cloudless, windless days within each period, five representative observation points were selected per plot between 10:00–14:00. A FieldSpec Pro FRTM spectrometer (Analytical Spectral Devices, USA) was used to measure canopy spectral reflectance. The instrument had a 25° field of view and spectral range of 350–2,500 nm, with 3 nm resolution and 1.4 nm sampling interval in the 350–1,000 nm range, and 10 nm resolution and 2 nm sampling interval in the 1,000–2,500 nm range. Standard whiteboard calibration was performed before each plot measurement, with the probe positioned vertically downward approximately 1.0 m above the rice canopy. Each observation point was measured five times, and the arithmetic mean of 25 spectra per plot was used as the final canopy spectral result, yielding 120 valid canopy spectral datasets across five growth stages and 24 plots. [Figure 1: see original paper] shows the canopy spectral reflectance trends under different nitrogen levels at the booting stage, with similar patterns observed at other key growth stages.

1.3.2 Determination of Leaf Chlorophyll and Carotenoid Content Chlorophyll (a+b) and carotenoid contents were determined using a mixed solution extraction method (acetone:anhydrous ethanol = 1:1), synchronized with canopy spectral measurements. Four representative plants were selected per plot, and equal numbers of upper, middle, and lower fully expanded leaves were collected, cut into pieces, and mixed uniformly. A 0.200 g sample was extracted with 50 mL of mixed solution at room temperature in darkness for approximately 24 hours until completely bleached, after which chlorophyll and carotenoid contents were measured using a spectrophotometer [15].

1.4 Data Analysis and Modeling

1.4.1 Data Preprocessing For pigment content estimation, only the 400–1,350 nm range with high signal-to-noise ratio was used as valid analytical data. To reduce noise, the Savitzky-Golay convolution smoothing method was applied with a moving window width of 15 and polynomial degree of 2. The measured pigment contents and corresponding canopy hyperspectral data were combined into an original dataset and randomly divided into two groups: 80 samples for model calibration and 40 samples for model validation.

1.4.2 Band Depth Analysis (BDA) Since leaf pigment content is primarily related to visible bands, depth analysis focused on the 400–750 nm spectral range, encompassing the strongly absorbing blue and red regions and the "red edge" band. First, continuum removal transformation was applied to spectral data to correct band-dependent shifts in reflectance extrema and effectively enhance absorption features while increasing differences among spectral curves

[10]. The "continuum line" was defined as line segments connecting local peaks in original spectral reflectance ([Figure 2: see original paper]). Continuum-removed reflectance (R) was obtained by dividing the spectral reflectance at each wavelength (R) by the corresponding continuum line value (Rc).

Four band indices were then calculated from continuum-removed spectra using the formulas in : band depth (BD), band depth ratio (BDR), normalized band depth index (NBDI), and band depth normalized to band area (BNA). These indices further reflect pigment absorption characteristics.

1.4.3 Modeling Method Principal component analysis (PCA) is a multivariate statistical method that reduces multiple variables to a few principal components through dimensionality reduction. PCA was applied separately to original bands (R), band depth (BD), band depth ratio (BDR), normalized band depth index (NBDI), and band depth normalized to band area (BNA). For consistency in subsequent BP neural network construction, the first 10 principal components were extracted for each, with cumulative contribution rates of 99.49%, 99.85%, 99.55%, 90.46%, and 99.97%, respectively. This reduced spectral dimensions from 351 to 10 while retaining most characteristic information, which were then input into the BP neural network model.

The BP neural network is a feedforward network comprising input, hidden, and output layers. The learning process involves forward signal propagation and error backpropagation. During forward propagation, input samples are processed layer-by-layer through neurons using S-type transfer functions from input to hidden to output layers. If actual output deviates from expected output, error backpropagation occurs, distributing output errors back through hidden layers to the input layer and adjusting weights to minimize error signals until meeting preset tolerance requirements [16].

With 10 principal components as input vectors, hidden layer node numbers were determined via trial-and-error to optimize nonlinear prediction performance, yielding 10 nodes for the carotenoid model and 11 nodes for the chlorophyll model. The single output layer represented rice leaf pigment content. Network training used 10,000 iterations, a training target parameter of 0.001, and a learning error of 0.01, with the L-M optimization algorithm (Trainlm) as the training function ([Figure 3: see original paper]).

1.4.4 Calculation of Pigment Spectral Parameters Based on established calculation methods, 17 widely recognized and relevant pigment spectral indices were selected () for linear and nonlinear model fitting to identify optimal pigment estimation models. Model performance was evaluated using coefficient of determination (R^2) and root mean square error of calibration (RMSEC) for modeling accuracy, and R^2, root mean square error of prediction (RMSEP), and relative percent deviation (RPD) for validation accuracy. R^2 reflects model stability and fit (closer to 1 indicates better stability and higher fit). RMSE and RPD evaluate model error and precision, with smaller RMSE indicating better

estimation capability. RPD > 1.4 indicates an acceptable model, while RPD > 2.0 signifies an excellent model [17]. All data processing was implemented using Matlab 2010b.

2 Results

2.1 Statistical Characteristics of Pigment Content

The calibration set had mean carotenoid content of 0.72 ± 0.24 mg $\cdot$ g^{-1}, while the validation set showed 0.71 ± 0.19 mg $\cdot$ g^{-1} (). For chlorophyll, the calibration set mean was 2.16 ± 0.79 mg $\cdot$ g^{-1} and the validation set mean was 2.21 ± 0.66 mg $\cdot$ g^{-1}. The small differences in means and low standard deviations between calibration and validation sets indicate good similarity, satisfying model development and validation requirements.

One-way ANOVA of leaf carotenoid and chlorophyll contents across growth stages and fertilization levels revealed that from tillering to jointing stages, carotenoid content differences among fertilization treatments were not significant, but became significant after booting. Chlorophyll content showed significant differences among nitrogen treatments at all growth stages. Both pigments followed similar trends: increasing from tillering to booting stage, decreasing markedly at heading, and showing lowest levels at filling stage ([Figure 4: see original paper]). From tillering to booting, leaf carotenoid and chlorophyll contents increased as plants continued vegetative growth and leaf development. From booting to filling, contents decreased as nutrients translocated to panicles and pigment synthesis weakened. During filling, leaf senescence and yellowing further reduced photosynthetic function and pigment synthesis.

2.2 Spectral Index Performance

2.2.2 Estimation Capability of Spectral Indices Using 17 representative spectral parameters, optimal prediction models for carotenoid and chlorophyll were constructed based on maximum fitting R^2 and compared with BDA-BP models (,). Carotenoid models showed moderate fitting (R^2 0.6, relatively small RMSE) but poor validation ($R^2 < 0.50$, RPD < 1.4). For chlorophyll, PRI, PSRI, and SIPI showed high fitting and validation accuracy ($R^2 > 0.60$, RPD > 1.4), making them suitable for chlorophyll estimation. Other indices produced unsatisfactory models with low validation accuracy, large RMSEP, and small RPD. These results indicate that pigment spectral index models cannot effectively estimate rice leaf carotenoid content, while vegetation indices using blue-red absorption and green peak reflectance bands (PRI, PSRI, SIPI) can better estimate leaf chlorophyll content.

2.2.3 Saturation Analysis of Spectral Indices for Different Pigment Contents [Figure 5: see original paper] shows scatter relationships between

carotenoid content and the more accurate indices (CTR2, PSSNRa, PSSNRb) and between chlorophyll content and high-performing indices (PRI, PSRI, SIPI). When carotenoid content exceeded 0.8 $mg \cdot g^{-1}$, scatter points for CTR2, PSSNRa, and PSSNRb showed random distribution. Similarly, when chlorophyll content exceeded 2 $mg \cdot g^{-1}$, scatter points for PRI, PSRI, and SIPI exhibited irregular patterns, indicating that at high pigment levels, hyperspectral parameters could not consistently reflect pigment content changes and showed fluctuating stability. Inflection points were identified from scatter plots to divide carotenoid content into two subsets: Subset I (< 0.8 $mg \cdot g^{-1}$, medium-low content) and Subset II (> 0.8 $mg \cdot g^{-1}$, high content). Chlorophyll was similarly divided into Subset I (< 2 $mg \cdot g^{-1}$) and Subset II (> 2 $mg \cdot g^{-1}$). Random selection of 40 samples from each subset for prediction showed that RMSE values increased with pigment content, indicating lower prediction accuracy for high-content samples and confirming saturation phenomena (). CTR2 (best correlated with carotenoids) and PRI (best correlated with chlorophyll) demonstrated higher prediction accuracy across different content levels than other indices.

2.3 Pigment Content Estimation Using BDA-BP Combination

demonstrates that BDA-BP models substantially improved estimation accuracy for both pigments and effectively overcame saturation problems. For carotenoid prediction, validation results for BD, BDR, and BNA showed higher R^2 and RPD but lower RMSE compared to original bands (R), indicating BDA outperformed raw spectral data in extracting pigment-related information. The BD-BP model achieved the highest calibration R^2 and, despite slightly lower validation R^2 than the BNA-BP model, showed the smallest RMSEP and largest RPD (1.67), making it optimal for rice leaf carotenoid estimation. For chlorophyll prediction, BDA also outperformed original bands, with the BNA-BP model achieving the highest calibration R^2 and, although validation R^2 was marginally lower than the BD-BP model, it produced the smallest RMSEP and largest RPD (1.91), making it optimal for total chlorophyll estimation ([Figure 6: see original paper], [Figure 7: see original paper]).

Compared with the best regression models based on spectral parameters, BDA-BP models significantly improved estimation precision for both pigments. Chlorophyll models consistently outperformed carotenoid models, likely because carotenoid and chlorophyll absorption peaks overlap and chlorophyll content is substantially higher than carotenoid content in leaves, making carotenoid estimation more challenging.

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3 Discussion and Conclusion

This study addressed the saturation problem in hyperspectral vegetation index inversion of rice leaf pigment content by combining band depth analysis

with BP neural networks. Compared with 17 spectral parameter-based models, this approach significantly improved estimation accuracy. Continuum removal transformation enhanced differences in spectral absorption characteristics, revealed more potential information, and strengthened discriminative features of spectral curves with varying pigment content, particularly in the red absorption valley where band depth features contain substantial pigment-related information [6]. Band depth analysis effectively reduces impacts from soil background, atmospheric scattering, and absorption, enabling more accurate estimation of leaf biochemical parameters [13] and addressing saturation issues in high-density vegetation areas [12].

Numerous studies confirm that relationships between vegetation biochemical parameters and canopy spectra are nonlinear due to weather, solar radiation, leaf geometry, soil background, and operational factors [30-31]. Neural networks offer significant advantages for fitting complex nonlinear problems and have become an important method for addressing such challenges. Vegetation indices suffer from saturation at high pigment levels, resulting in low estimation accuracy. The BDA-BP models developed in this study effectively resolved saturation problems by leveraging complementary information across different bands beyond the limitations of individual vegetation indices, thereby improving estimation precision.

Band depth analysis of visible bands followed by PCA dimensionality reduction effectively preserved information, enhanced network performance, prevented overfitting, and improved pigment content inversion accuracy. However, this study focused on a single cultivar under controlled plot conditions. Further validation across different regions and cultivars is needed. Radiative transfer models offer greater universality, and future work should develop empirical-physical coupled models [34] to further improve accuracy and applicability. Integration of these models with spatial remote sensing information at larger scales will provide theoretical and practical references for regional rice leaf pigment content estimation.

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Note: Figure translations are in progress. See original paper for figures.