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Available online: 24 Feb 2010


To link to this article: http://dx.doi.org/10.1080/01431160902912061

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Evaluating the performance of PC-ANN for the estimation of rice nitrogen concentration from canopy hyperspectral reflectance

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(Received 31 May 2008; in final form 19 March 2009)

In this study, a wide range of leaf nitrogen concentration levels was established in field-grown rice with the application of three fertilizer levels. Hyperspectral reflectance data of the rice canopy through rice whole growth stages were acquired over the 350 nm to 2500 nm range. Comparisons of prediction power of two statistical methods (linear regression technique (LR) and artificial neural network (ANN)), for rice $N$ estimation (nitrogen concentration, mg nitrogen g$^{-1}$ leaf dry weight) were performed using two different input variables (nitrogen sensitive hyperspectral reflectance and principal component scores). The results indicated very good agreement between the observed and the predicted $N$ with all model methods, which was especially true for the PC-ANN model (artificial neural network based on principal component scores), with an RMSE = 0.347 and REP = 13.14%. Compared to the LR algorithm, the ANN increased accuracy by lowering the RMSE by 17.6% and 25.8% for models based on spectral reflectance and PCs, respectively.

1. Introduction

Among the many foliar chemicals, nitrogen is an important indicator of photosynthetic rate and overall nutrition status (Curran 1989). Many studies in precision farming are focused on nitrogen rate and timing for high yield, crop quality and environment pollution control (Smil 1997). Tools that can rapidly quantify the nitrogen status of crops in large areas are needed for efficient fertilizer management.

Previous studies have demonstrated the great potential of remote sensing techniques to rapidly evaluate the $N$ variability over large fields (LaCapra et al. 1996, Martin et al. 2005), and several statistical strategies have been used to analyse the relationship between vegetation biochemicals and remote sensing data. Among those statistical methods, stepwise multiple linear regression (SMLR) analysis was the most widely used (Shibayama and Akiyama 1991, Grossman et al. 1996). In recent years, quantitative remote sensing of vegetation biochemicals has advanced due to the use of multivariate statistical methods, particularly artificial neural networks (ANN) (Dou et al. 2006). The ability of ANN to associate complex spectral information with target attributes without any constraints on the sample distribution (Mather 2000) make
them ideal for describing the intricate and complex nonlinear relationships that exist between canopy-level spectral signatures and various crop conditions (Kimes et al. 1998, Lillesand and Kiefer 2000). In fact, applications have already been reported for soil moisture estimation (Frate et al. 2003) and biomass estimation (Jin and Liu 1997). However, few attempts have been made so far to examine the potential of combining the properties of ANN with principal component analysis (PCA), i.e. in the PC-ANN model (artificial neural network model based on principle component scores), for the estimation of rice leaf nitrogen concentration from canopy-scale hyperspectral reflectance. In this study, a first attempt is made. The aim of this study is (1) to evaluate the potential of PC-ANN for the estimation of rice $N$ from canopy hyperspectral reflectance, and (2) to compare the capabilities of LR and ANNs.

2. Materials and methods

2.1 Experimental design

A field experiment was carried out during June–October 2004 at Zhejiang University Experiment Farm, Hangzhou, Zhejiang Province, China, located at 30° 14' N, 120° 10' E. The sandy loam paddy soil had the following properties: pH 5.7, 16.5 mg g$^{-1}$ organic matter and 1.02 mg g$^{-1}$ total $N$. To obtain sufficient variation in nitrogen concentration levels, two cultivars of rice, i.e. Xieyou 9308 (erectophile) and Xiushui 110 (planophile), which were significantly different in leaf orientation, were grown in 18 plots with three nitrogen fertilization treatments: 0, 140 and 240 kg ha$^{-1}$ pure nitrogen. Every treatment had three repetitions.

2.2 Measurements of canopy spectral reflectance

Canopy spectral readings and corresponding nitrogen concentration measurements were performed six times, which corresponded to early tillering stage, peak tillering stage, gestation stage, heading stage, milky stage and ripening stage, respectively. Canopy reflectance was obtained using an Analytical Spectral Devices, FieldSpec Full Range (ASD FieldSpec FR, ASD, Inc., Boulder, CO, USA) that acquires continuous spectra from 350 nm to 2500 nm. All canopy spectral measurements were taken on a clear day with no visible cloud cover between 10:00 am and 14:00 pm (Beijing local time). In each plot, representative plants were selected for canopy spectral measurement. The sensor head was placed approximately 1.0 m vertically above canopies with a 25° field of view. The reflectance of a white Spectralon (BaSO$_4$) panel was measured before every crop reflectance measurement, and crop reflectance was then calculated as the ratio between energy reflected by the crop and energy incident on the crop, (i.e. solar irradiation), which used measurements of the white Spectralon (BaSO$_4$) reflectance panel. Every crop reflectance measurement was an average of 10 repeated scans that were acquired automatically by the FieldSpec.

2.3 Measurements of nitrogen concentration

Green plant sampling was performed almost simultaneously with every canopy spectral measurement. After spectral measurements, plant samples were cut immediately and placed in plastic bags and transported to the laboratory for subsequent analysis. Leaf nitrogen concentration was determined by Kjeldahl and the results were expressed in mg N g$^{-1}$ leaf dry weight. The samples were divided randomly into a calibration set and a validation set. The descriptive statistics of $N$ values for model
calibration and validation are summarized in Table 1. A wide range of leaf total nitrogen concentration levels was established, with the maximum value of 4.82 and the minimum value of 0.91, which ensured the relationship between $N$ and reflectance measurements as realistic and universal as possible.

### 2.4 Artificial neural network

An ANN is a multi-layer weighted-node connectionist architecture that learns through training. Of all the artificial neural networks, the back-propagation algorithm is perhaps the most widely used supervised training algorithm for multilayered feed-forward networks. Successful application of a back-propagation network to the estimation of biomass and nitrogen concentration has been made (Goel et al. 2003). The back-propagation algorithm was also adopted for ANN analysis in this study. A brief discussion of NNs can be found in Keiner and Yan (1998).

### 2.5 Principal component analysis

PCA is an important method for data reduction, summation and representation. The main purpose of PCA is to build linear combinations of the original variables that represent the most variations of the original dataset (Manly 1994, Ceballos and Bottino 1997).

In this letter, PCA is performed on the calibration and validation canopy hyperspectral reflectance for wavelength ranges 350–1350 nm, 1450–1800 nm and 1950–2400 nm. A number of procedures are used to compute scores (Harman 1967, Wahlstedt and Davis 1968, Davis 1973). Components are based on the covariance matrix, and eigenvectors are scaled by square roots of their eigenvalues. The detailed process for score computation will not be described in this letter, but further information on the method can be obtained in Trochimczyk and Chayes (1978).

### 2.6 Criteria for model performance evaluation

The performances of models were measured by coefficient of determination of the model ($R^2$), the root mean square error (RMSE) (Kvalheim 1987) and the relative error of prediction (REP). For the calculation of RMSE and REP see Yi et al. (2007). The smaller RMSE and REP indicate the better performance of models.

### 3. Results

#### 3.1 Characteristics of canopy spectral reflectance and analysis of correlation between spectra and nitrogen

As expected, reflectance spectra of the canopy were significantly different among growth stages throughout most of the wavelengths measured (figure 1). Spectral
differences among different growth stages in the red and blue bands were more obvious than those among different fertilization treatments, and the most obvious changes were found in the near-infrared region.

The relationships between the spectra of the rice canopy at different growth stages and nitrogen concentration are illustrated in figure 2. Absolute values of correlations in the near-infrared region were generally larger than those in visible regions.

Figure 1. Average reflectance of rice canopy at different growth stages.

Figure 2. Coefficients of correlation relating the spectral reflectance of the rice canopy at different growth stages to nitrogen concentration.
Compared to correlations at other growth stages, correlations between spectra at the early tillering stage and nitrogen concentration were much smaller throughout the visible and infrared regions.

### 3.2 Results of principal components analysis

The cumulative variances of the first five principal components for the calibration dataset and validation dataset are summarized in Table 2. It was found that 99.03% and 98.79% of the variance respectively included in the total 1803 input variables of calibration data and validation data could be explained by the first five principal components, while the other principal components contained less information. Thus, for model development, factor scores, calculated from the first five principal components, were used as the input variables for the PC-ANN and PC-LR modelling methods.

### 3.3 Model development

It was noted that due to severe noise in the water absorption spectrum at 1350–1450 nm and 1800–1950 nm, the effective rice canopy hyperspectral reflectances for wavelength ranges 350–1350 nm, 1450–1800 nm and 1950–2400 nm were used in the development of different models. For all models, 121 samples out of 201 samples were used for model calibration and the remaining 80 samples were used to examine the validity of the models.

#### 3.3.1 Results of linear regression modelling

Two different input strategies were used for the development of LR models. In the first strategy, all spectra were used directly as independent to conduct SMLR. The stepwise criteria were: $p < 0.05$ for entry and $p > 0.10$ for removal. Through analysis, the coefficient of determination ($R^2$) of the five-regressor model has reached a significant level, with the value of 0.801. Beyond the fifth regressor, the increase in $R^2$ of models with every addition of another regressor became small. Thus, in this study, the maximum number of independent variables in the model was set to five.

The first five wavelengths selected by SMLR were located at 351 nm, 673 nm, 679 nm, 2073 nm and 2236 nm, and many of the absorption features are known nitrogen absorption features. For example, 673 nm and 679 nm correspond to a chlorophyll absorption feature that is closely related to N, and 2073 nm and 2236 nm correspond to N absorption features identified by Lee (2001), while 351 nm does not fall in the absorption region for N. Those five selected bands were also used as inputs for the PC-ANN for the estimation of rice nitrogen concentration.

### Table 2. Percentage of explained variance for the first five PCs. PC1 and PC2 capture the most significant information contained in the spectral reflectance variation.

<table>
<thead>
<tr>
<th></th>
<th>PC1</th>
<th>PC2</th>
<th>PC3</th>
<th>PC4</th>
<th>PC5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibration</td>
<td>Explained variance (%)</td>
<td>64.72</td>
<td>30.55</td>
<td>2.28</td>
<td>1.05</td>
</tr>
<tr>
<td></td>
<td>Cumulative variance (%)</td>
<td>64.72</td>
<td>95.27</td>
<td>97.54</td>
<td>98.59</td>
</tr>
<tr>
<td>Validation</td>
<td>Explained variance (%)</td>
<td>69.57</td>
<td>23.36</td>
<td>3.71</td>
<td>1.41</td>
</tr>
<tr>
<td></td>
<td>Cumulative variance (%)</td>
<td>69.57</td>
<td>92.93</td>
<td>96.64</td>
<td>98.05</td>
</tr>
</tbody>
</table>
input variables in R-ANN model (artificial neural network based on sensitive hyperspectral reflectance).

In the second strategy, factor scores of the first five principal components were used as independent variables to conduct regression. Equations of two resultant LR models are presented in table 3.

### 3.3.2 Results of artificial neural network modelling.

ANN models were obtained with MATLAB (version 6.5). The backpropagation algorithm was employed to train the neural network. Two different ANN models with two different input variables, namely five reflectance variables selected by SMLR technique and factor scores of the first five principal components, were tested. In both ANN models, a three-layer network architecture, consisting of one input layer, one hidden layer and one output layer, was established and a hyperbolic tangent sigmoid transfer function was used at the input layer and the hidden layer and a pure line transfer function was used at the output layer. The Levenberg-Marquardt training algorithm was used for training the network. The number of neurons for the input layer was equal to the number of input variables introduced in the networks. The output layer contained one neuron. The proper number of neurons in the hidden layer was determined by training the ANN with different numbers of neurons in the hidden layer and computing the correlation coefficient between the output target and the simulated value of the target, and the optimum number of neurons in the hidden layer was determined when the maximum value of correlation coefficient was obtained. After a time-consuming trial, an R-ANN model, with a 5-9-1 architecture and a PC-ANN model with a 5-11-1 architecture, was selected.

### 3.4 Model performance comparison

The $R^2$, RMSE and REP calculated with the calibration and validation datasets for all models are summarized in table 4. It can be concluded from the table that compared to the conventional liner regression method, the artificial neural network algorithm gave the maximum $R^2$ values, and the lowest RMSE and REP. The largest $R^2$ (0.944), and the smallest RMSE (0.249) and REP (9.48%) for the calibration dataset, and the largest $R^2$ (0.895), and smallest RMSE (0.347) and REP (13.14%) for the validation dataset were all obtained by PC-ANN, and followed by the R-ANN model, R-LR model and PC-LR models.

Performance comparisons between models using different model methods but the same input variables showed that in both cases the prediction power of models obtained by ANN modelling was greater than that obtained by LR technique. As can be seen, compared to the two LR models the corresponding ANN models, i.e. R-ANN and PC-ANN, respectively increased the prediction of $N$ by lowering

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**Table 3. Equations for two linear regression models.**

<table>
<thead>
<tr>
<th>Methods</th>
<th>Model expressions</th>
</tr>
</thead>
<tbody>
<tr>
<td>R-LR</td>
<td>$N = 1.857 + 80.902R_{351} - 1931.88R_{673} + 1907.44R_{679} - 64.73R_{2023} + 27.91R_{2236}$</td>
</tr>
<tr>
<td>PC-LR</td>
<td>$N = 2.66 - 0.0003PC_1 - 0.00097PC_2 - 0.01126PC_3 + 0.02826PC_4 - 0.0005PC_5$</td>
</tr>
</tbody>
</table>

$N$ is nitrogen concentration; $R_i$ indicates reflectance value at the $i$th wavelength (nm); $PC_i$ indicates the principal component of the $i$th level.
RMSE by 17.6% and 25.8%, and REP by 6.7% and 9.79% for the calibration dataset, and RMSE by 2.6%, 4.3%, 2.2% and 19.7% and REP by 0.83%, 2.63%, 1.18% and 7.44% for the validation dataset. In addition, compared to the R-ANN model, PC-ANN perfected the results by lowering RMSE by 4.6% and 17.8% and REP by 1.73% and 6.74% for the calibration and validation datasets, respectively.

In order to make the comparison of results more convincing and visual, the observed $N$ against the predicted $N$ obtained by estimation models is plotted in figure 3. Ideally, the 1:1 line should be a perfect match. The efficiency of the PC-ANN model is evident from the figure; the regression line between the observed and the predicted $N$ nearly overlaps the 1:1 line, which is the case for both calibration and validation sets. Additionally, comparing the predictive capability of ANN and LR methods, it is clear that the results obtained by the ANN modelling method are more accurate than the linear regression method.

### 4. Discussion and conclusions

In the present study, nitrogen concentration was estimated using two methods (LR and ANN), and two input variables (spectral reflectance and scores of the first five principal components). The results showed that the ANN method has the potential to perfect the estimation of $N$ concentration. Through analysis, it was found that estimating leaf $N$ concentration by the ANN method was generally more accurate than by the LR method when the same input variables were used, which indicated that the ANN should be a much more efficient method compared to LR. This is especially true when the ANN method was combined with PCA. The PC-ANN model performed significantly more accurately than other models in all cases. Moreover, the ANNs gave an unbiased prediction, while other methods systematically under- or over-predicted $N$. The promising potential of the PC-ANN algorithm used as an exploratory and predictive tool was identified in this study.

This study was the first attempt to estimate leaf $N$ concentration using ANN combined with PCA and canopy-scale hyperspectral reflectance. However, some problems should be discussed. For ANNs, the process of finding the best result is complicated and it cannot be guaranteed that the reported result is the optimum because an exhaustive search is excessively time-consuming and there are no well established rules to determine the best network architecture and training methods. All neural network results reported in this letter were trained based on experience by testing a limited number of combinations. In general, we varied the number of hidden

<table>
<thead>
<tr>
<th>Methods</th>
<th>$R^2$</th>
<th>RMSE</th>
<th>REP</th>
<th>$R^2$</th>
<th>RMSE</th>
<th>REP</th>
</tr>
</thead>
<tbody>
<tr>
<td>R-LR</td>
<td>0.801</td>
<td>0.471</td>
<td>17.91</td>
<td>0.775</td>
<td>0.494</td>
<td>18.70</td>
</tr>
<tr>
<td>R-ANN</td>
<td>0.925</td>
<td>0.295</td>
<td>11.21</td>
<td>0.753</td>
<td>0.525</td>
<td>19.88</td>
</tr>
<tr>
<td>PC-LR</td>
<td>0.769</td>
<td>0.507</td>
<td>19.27</td>
<td>0.744</td>
<td>0.544</td>
<td>20.58</td>
</tr>
<tr>
<td>PC-ANN</td>
<td>0.944</td>
<td>0.249</td>
<td>9.484</td>
<td>0.895</td>
<td>0.347</td>
<td>13.14</td>
</tr>
</tbody>
</table>

$R^2$: coefficient of determination; RMSE: root mean square error; REP: relative error of prediction (%).
Figure 3. Scatterplots of observed versus predicted nitrogen concentration. (a) Calibration data; (b) validation data. The dashed line represents the 1:1 line, and the solid line represents the regression line.
neurons to find the best result, and reported the method that gave the highest correlation coefficient. Although satisfactory results were obtained with the ANN algorithm, and its capabilities were proved superior to traditional model methods, these two fields may mutually assist each other to obtain a more accurate result. Also, the results presented in this work were obtained for only two rice cultivars, grown under controlled conditions. In this respect, further experiments are needed to clearly identify the effectiveness of the PC-ANN technique.

Acknowledgements
The assistance given by colleagues in Institute of Agricultural Remote Sensing & Information Technology is highly appreciated. Financial support was received from the programme of National Natural Science Foundation of China under Grant No. 40571115.

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