 DOI: 10.3217/978-3-85125-954-4-16

Estimation of nitrogen yield in wheat using radiative transfer model inversion based on an artificial neural network

L. J. Koppensteiner
Institute of Agronomy, BOKU
Konrad Lorenz-Straße 24, 3430
lukas.koppensteiner@boku.ac.at

R. W. Neugschwandtner
Institute of Agronomy, BOKU
Konrad Lorenz-Straße 24, 3430
reinhard.neugschwandtner@boku.ac.at

Abstract

The objective of this study was to estimate nitrogen yield in wheat based on hyperspectral reflectance measurements with a handheld spectroradiometer. To do so, the radiative transfer model PROSAIL was inverted and an artificial neural network applied. The model was trained and tested using a simulated dataset and field experimental data. Results of the simulated dataset show that the inversion of PROSAIL based on an artificial neural network was successful. Furthermore, estimations of nitrogen yield compared to experimentally collected data feature high R^2 and low RRMSE. The technique proposed in this study is a promising tool to collect information on nitrogen yield of wheat canopy in a quick and non-destructive way with low calibration requirements. This can be utilized by practical farmers for field monitoring and site-specific nitrogen fertilization as well as scientists and breeders for quick and non-destructive data collection in field experiments. Additionally, this approach can be adapted for different crops and varying sensors, e.g., multi- and hyperspectral UAV-mounted sensors as well as satellite data.

1. Introduction

Remote sensing allows quick and non-destructive measurements of canopy characteristics. Commonly, vegetation indices are applied, however, this approach usually requires continuous calibration and cannot use all available spectral data for analysis. Radiative transfer models (RTMs) are a promising alternative to vegetation indices. These models describe the interaction between solar radiation and vegetation canopy [1]. Compared to vegetation indices, RTMs generalize well, have low calibration needs and allow analysis of all available spectral data [2].

The objective of this study was to estimate nitrogen yield in wheat (*Triticum aestivum* L.) using an artificial neural network-based inversion of the RTM PROSAIL.

2. Materials and methods

The RTM PROSAIL simulates the spectral reflectance of vegetation canopy from 400 to 2500 nm in 1 nm increments using information on leaf characteristics, canopy architecture, viewing geometry and other effects (Figure 1). Simulations in the RTM PROSAIL (version 5B) were conducted using the package hsdar (version 1.0.3) in R programming language (version 4.1.1).

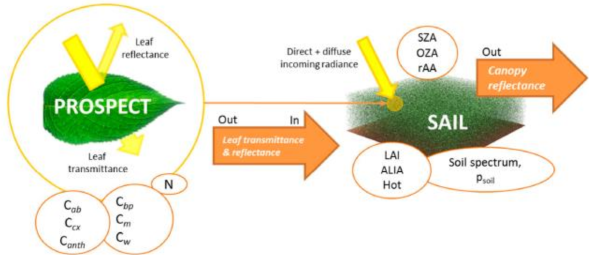

Figure 1: Calculation of canopy reflectance using the coupled PROSPECT + SAIL model (PROSAIL) [2]. N: leaf structure index (unitless). C_{ab}: chlorophyll a + b content (µg cm^{-2}), C_{cx}: carotenoid content (µg cm^{-2}), C_{anth}: anthocyanin content (µg cm^{-2}), C_{bp}: brown pigment content (unitless), C_m: dry matter content (g cm^{-2}), C_w: water depth (mm), LAI: leaf area index (m^2 m^{-2}), ALIA: average leaf inclination angle (°), Hot: hot-spot parameter (m m^{-1}), soil spectrum (% reflectance), p_{soil}: soil brightness factor (unitless), SZA: sun zenith angle (°), OZA: observer zenith angle (°) and rAA: relative azimuth angle (°).

A simulated dataset consisting of 100 000 observations was created for model training and testing. Each observation included a random set of PROSAIL input parameters drawn from uniform distributions of the PROSAIL input parameters within wheat-specific ranges from literature [3, 4]. Furthermore, spectral reflectance for background soil was varied among observations in the simulated dataset. To do so, available data on soil reflectance by the ICRAF-ISRIC Soil MIR Spectral Library of the International Soil Reference and Information Centre (ISRIC) were used [5]. The simulated dataset was divided into a train and test set in a 9:1 ratio.

Field experiments were conducted at the Experimental

Farm Groß-Enzersdorf of the University of Natural Resources and Life Sciences, Vienna, in the seasons 2019/20 and 2020/21. Data on nitrogen yield (NY, g m^{-2}) were collected in approximately 14-day intervals from March until harvest in July in both seasons. Destructive plant sampling was conducted on 0.6 m^2 per plot. Plant material was dried, weighed, milled and analyzed for N concentration according to the Dumas combustion method [6] using an element analyzer (vario MAX cube CNS, Elementar Analysensysteme, Germany). Resulting N concentration values were multiplied by above-ground dry matter to calculate NY. Measurements on canopy reflectance in the field experiment were conducted with the spectroradiometer FieldSpec Handheld 2 (ASD Inc., USA). This sensor provides hyperspectral reflectance data from 325 to 1075 nm in 1 nm increments.

An artificial neural network (ANN) was set up to achieve the inversion of the radiative transfer model PROSAIL. Model inputs were viewing geometry, background soil reflectance and canopy reflectance from 400 to 1075 nm in 1 nm increments. The spectral resolutions of soil reflectance, simulated PROSAIL canopy reflectance and spectral measurements from the field experiments were matched. Model outputs were the PROSAIL parameters N, C_{ab}, C_{cx}, C_{bp}, C_m, C_w, LAI, ALIA and Hot. The ANN consisted of three dense layers with 128 neurons each, ReLU activation function, loss function “mean absolute error” and optimizer “Adam”. Training epochs were set to a maximum of 500 with early stopping at 50 to avoid overfitting. Google Colaboratory, an available Keras implementation (version 2.8.0) in Python (version 3.6), was used to set up the ANN. Experimentally measured NY was estimated using predictions of $C_{ab} \times$ LAI. The model performance was evaluated using the simulated test dataset and field experimental data.

The accuracy of model predictions compared to measured values was evaluated using regression coefficients and coefficients of determination (R^2) in regression analysis. Furthermore, root mean square error (RMSE) and relative root mean square error (RRMSE) were calculated for model testing.

3. Results

Figure 2 presents the results of predicted LAI and C_{ab} compared to true values in the simulated test dataset. The parameters LAI and C_{ab} show high R^2, i.e., above 0.9, and low RRMSE (LAI: 17.3%, C_{ab}: 8.5%).

The relationship between measured and predicted C_{ab} is linear, while LAI shows a quadratic fit. When LAI was 0 m^2 m^{-2}, C_{ab} could not be estimated. For observations with LAI below 0.5 m^2 m^{-2}, C_{ab} predictions show slight underestimation at high C_{ab}.

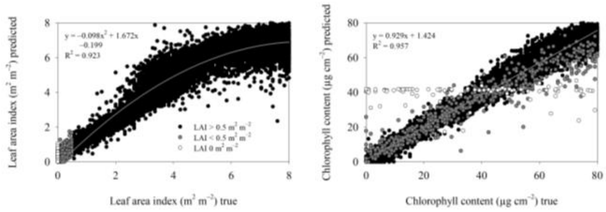

Figure 2: Estimation of leaf area index (left, m^2 m^{-2}) and chlorophyll content (right, µg cm^{-2}) of the simulated test dataset.

Predicted $C_{ab} \times$ LAI was calibrated using experimental data on NY from 2020/21. The calibrated predictions of NY were validated using experimental data from 2019/20 (Figure 3). In both seasons, R^2 values were high, i.e., above 0.8. In the experimental validation data of 2019/20, the deviation from the 45° line was low. At high NY, predictions show a slight underestimation.

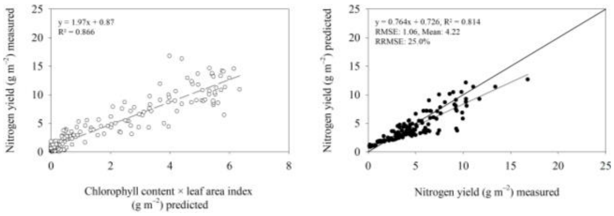

Figure 3: Calibration of predicted chlorophyll content × leaf area index (left, g m^{-2}) with measured nitrogen yield (g m^{-2}) of the field experiment in 2020/21 as well as validation of calibrated predictions on nitrogen yield (right) with respective measurements of the field experiment in 2019/20.

4. Discussion

Results on predicted LAI and C_{ab} based on the simulated test dataset showed, that the ANN based inversion of the RTM PROSAIL was successful. The quadratic relationship between true and predicted LAI indicates, that LAI estimations saturate at high values, i.e., above 4 m^2 m^{-2}. No leaf area is present for observations with LAI = 0 m^2 m^{-2}. As a result, leaf characteristics, such as C_{ab}, cannot be estimated. When LAI is low, e.g., below 0.5 m^2 m^{-2}, the effect of background soil on reflectance measurements is large and thus affects the estimation of leaf characteristics. This results in an underestimation of high chlorophyll concentrations, when LAI is low.

Results on estimations of $C_{ab} \times$ LAI compared to measured NY are promising, because of their high R^2 in both seasons as well as the low deviation from the 45° line and the low RRMSE of experimental validation data in 2019/20. This indicates high predictability of NY based on our model as well as high stability among seasons.

Acknowledgments

This work was supported by the project “DiLaAg – Digitalization and Innovation Laboratory in Agricultural Sciences” of the private foundation “Forum Morgen, Austria” and the Federal State of Lower Austria.

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