Reflecting on hyperspectral imaging: multiple strategies to model Nitrogen status in maize leaves

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ABSTRACT

Hyperspectral imaging is a promising method to predict traits in a high-throughput manner with the potential to unlock quantitative genetic studies. Researchers have successfully modeled physiological traits such as vegetative Nitrogen content, but scope of methodology and lack of truly novel testing data hinder large scale trust in the process. Here, I explore the ability to model leaf Nitrogen content from hyperspectral reflectance data collected with a LeafSpec imaging device on 22 maize hybrids. Three broad strategies based on different input feature sets are undertaken. Strategy one mines data for the most informative hyperspectral channels and then constructs a normalized index similar to NDVI as input features. Strategy two considers all 364 channels of hyperspectral data and makes predictions using various machine learning techniques; partial least squares regression(PLSR), random forest regression, and a feed-forward neural net regression. Strategy three aims to take advantage of the spatial distribution of hyperspectral data on the leaf surface by training a convolutional neural net(CNN). A normalized visual index constructed from bands most correlated with nutrient content out-performed established NDVI. PLSR was the most accurate algorithm, followed by feed-forward neural net and then CNN, based on coefficient of determination score. PLSR is well established as a robust method for hyperspectral prediction which is further evidenced by this study. This is one of the first applications of CNN for hyperspectral data. Despite not being the most accurate algorithm there remains room for hyper-parameter optimization.

Keywords: Hyperspectral, Machine Learning, Neural Network, Maize, Image processing, Nutrient, Vegetative

1. INTRODUCTION

There is variation in the wavelengths and intensity of light that is reflected by a corn leaf. The variation depends in part on the physiological state of the plant[1]. It is possible to capture specific wavelengths and intensities of light interacting with vegetative matter with hyperspectral imaging(HSI) technology. Many different biochemical and physical phenotypes of corn have been predicted using HIS such as plant water status[2], Nitrogen status[3, 4], and chlorophyll content[5] but limited testing of models with truly exclusive genotypes and development stages not shown during model training limits their application for plant breeding programs.

There are generally two different strategies so far to make predictions based on hyperspectral data. The first strategy is to take advantage of the breadth of wavelength channels captured by HSI, often 450 nm up to 2500nm, or 2000 possible input features (2500 – 450 = 200). Machine learning algorithms excel at translating large numbers of input features into quantitative predictions, with partial least squares regression(PLSR) being one of the most successful for HSI in particular[6]. Alternatively, a data scientist may preferentially select individual wavelengths and calculate ratios between the two such as the Normalized Differential Vegetative Index[6]. One aspect that both strategies ignore is the spatial distribution of wavelength intensities across the surface of a leaf. Both whole-spectra and index-based strategies currently, only consider the average intensity value across the leaf surface. It is well known that Nitrogen stress in particular appears as specific visual patterns on a maize leaf which is characterized by the vegetative tissue near the tip and midvein turning yellow first and growing down and out towards the base[7].

Using the Leafspec device it is possible to produce hyperspectral scans of a leaf that preserves spatial information in a 2d plane[8]. Further, it is well known that convolutional neural network is a powerful type of neural network that passes a small filter iteratively over the dimensions of an image and calculates a value based on a pixel and its neighbors. The result is that spatial features can be mapped to filters and inform modeling[CITATION]. To push the boundaries of HSI prediction in the plant sciences, I will construct a train and test set that are genotypically and developmentally distant from each other, representing truly new data to the models. In addition, I will thoroughly compare a broad stroke of strategies used for prediction ranging from simple 3-parameter linear regression to neural networks that contain millions of parameters.

2. MATERIALS AND METHODS

2.1 Plant material and data collection

Leafspec scans and total N content were acquired from either the ear leaf or 2nd top collard leaf depending on development stage(V6 – R3). Collections were made in 2020 and 2022 at two different fields in Central Michigan. Between two and five scans were taken per plot. Congruently, three to nine leaves were collected for total Nitrogen by dry weight percentage per plot. The testing set consists of scans and N for 22 hybrids(including the five) at approximately the R2 development stage in 2020. This represents approximately 28% of total samples, a new development stage, and 18 new hybrids not processed in training.

2.1 Model creation

NDVI calculated as, $NDVI = \frac{R800nm - R650nm}{R800nm + R650nm}$ where R800nm and R650nm are the reflectance values of the 800nm and 650 nm wavelengths. CorNDVI calculated as Cor$NDVI = \frac{R905nm - R569nm}{R905nm + R569nm}$. Linear regression, PLSR, and RF implemented in Sklearn. Feed forward neural network(FFNN) and convolutional neural network(CNN) implemented in Pytorch. Data tensors of resized CorNDVI images (1x234x234) were generated from (364x234x234) HIS cubes by calculating CorNDVI at every leaf pixel. CNN Architecture used in this study involved a single convolution kernel of size (4x4), followed by ReLU activation and a maxpool layer of size (4x4) fed into a 2-layer linear network to regression. The CNN was trained for 500 epochs.

3. RESULTS

3.1 Normalized index approach

Index-based methods are the simplest strategy. NDVI and a custom normalized index, henceforth referred to as CorNDVI, was constructed for comparison. CorNDVI was calculated from two total wavelengths near the red and infrared zones with the strongest correlation values to Nitrogen concentration (Figure 1.) NDVI and CorNDVI were both used in a simple linear model to predict N status and CorNDVI outperformed traditional NDVI(Table 1.).

3.2 Whole spectra, machine learning approaches

Three different machine learning algorithms were employed to leverage the wide breadth of wavelengths captured by HSI and determine if modelling accuracy could be improved by greatly increasing the number of input features. Hyperparameter tuning was done for each method. The optimum PLSR fit was achieved with 4 latent variables. Random Forest(RF) regression was optimized for 250 estimators. The feed-forward neural net was optimized for layer architecture. A deeper network(more layers) performed better than a wide layout(more nodes). PLSR and the neural network performed better than CorNDVI but RF did not(Table 1).

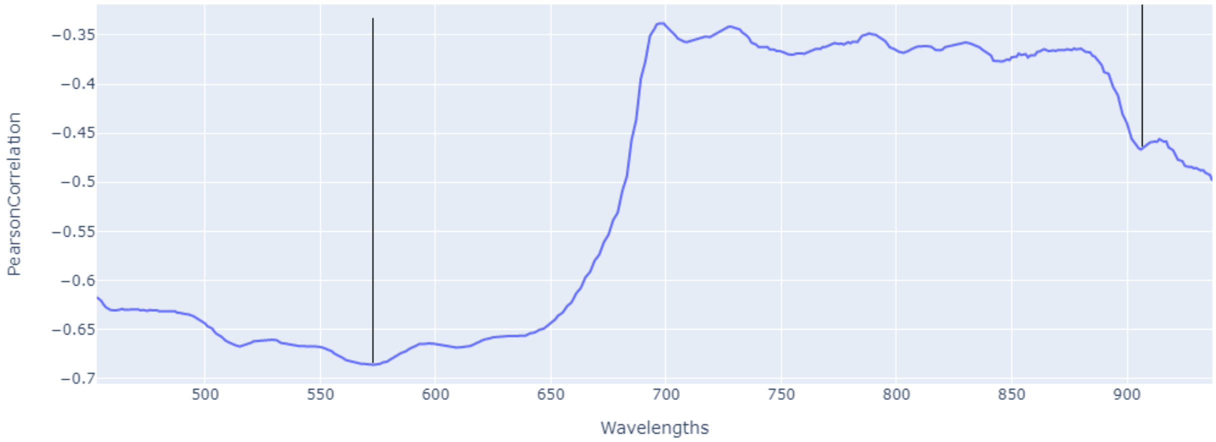

Figure 1. For each wavelength from 453nm to 937 nm the Pearson's Correlation value was calculated between that wavelength and Nitrogen content. All correlations were negative. Channels 569nm and 905nm(black bars) were selected to calculate custom index.

3.3 Convolutional Neural Net approach

To explore the usefulness of spatial hyperspectral intensity information a CNN pipeline was established. First images had to be resized to common dimensions of 234 pixels tall by 234 pixels wide by 364 channels of wavelengths (234x234x364). In order to make the computational resources for CNN more palatable the (234x234x364) matrix was resized to a single channel so the final input for training was (234x234x1). A CorNDVI image was used as the one channel due to its ability to predict N status more effectively than NDVI. Preliminary visualization of CorNDVI heatmaps suggest that high N status leaves have a visual banding pattern which is absent from low N status plants.(Figure 2).

4. DISCUSSION AND CONCLUSION

The testing set used in this study was intentionally made challenging by introducing novel hybrids and time point for prediction. Positive results indicate that robust models can probably be built up to process new input data for N concentration. The data driven procedure to build CorNDVI showed a better indicator than conventional NDVI for N status and may represent an acceptable approach to build other prediction algorithms. CorNDVI linear regression outperformed RF regression at a fraction of the computational cost indicating that a few informative wavelengths may be sufficient to generate accurate predictions. PLSR has been shown as one of the most powerful machine learning techniques for hyperspectral data and the results here agree because it was the best performer. However, there remains room to optimize parameters of CNN such as the number of channels and filters. In this study, the number of channels was simplified to 1, from 364 to reduce computational cost but cloud-computing infrastructure may allow more parameters to be trained. Continued work will be needed to determine whether predictions can be improved on further with a CNN approach.

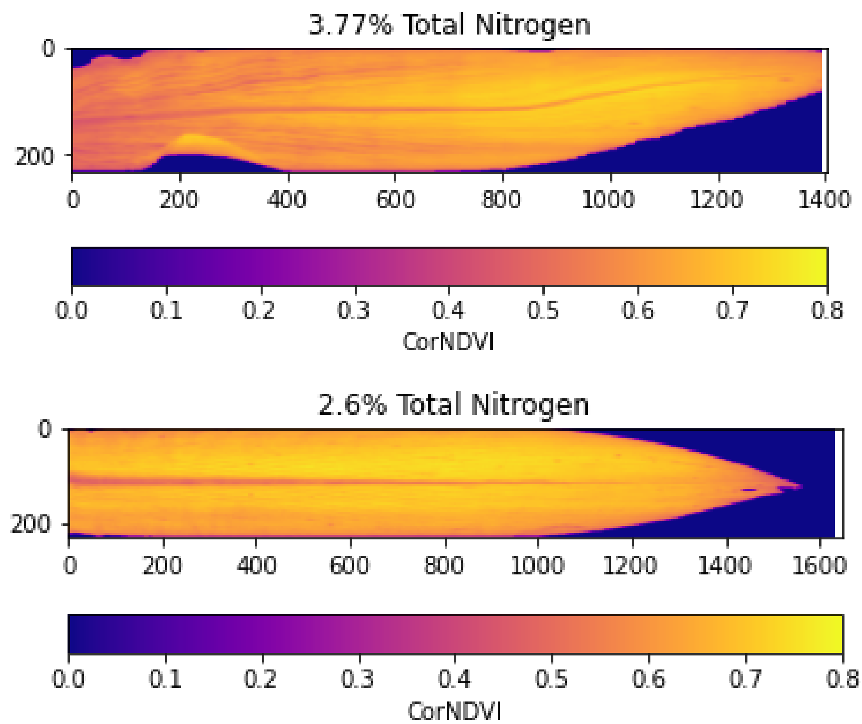

Figure 2. CorNDVI heatmaps of two leaves taken from the same plot. High N status is shown top and low N status shown bottom. The high N status leaf with clear banding running parallel to the mid vein that is absent in low N status leaf.

Table 1. Model results from various strategies to predict percent Nitrogen status in test set of samples. PLSR – partial least squares regression. RF – random forest regression. FFNN – Feed-forward neural network. CNN – Convolutional neural network.

Strategy	Prediction goodness of fit - R^2	Prediction mean square error (% Total Nitrogen)
NDVI_Regression	0.21	0.21
CorNDVI_Regression	0.41	0.16
PLSR	0.57	0.12
RF	0.39	0.16
FFNN	0.54	0.12
CNN	0.49	0.14

DATA AVAILABILITY STATEMENT

CorNDVI tensors and scripts are available at https://github.com/B-Webster-Bio/NuteNet

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REFERENCES

[1] Kumar, L., Schmidt, K., Dury, S., Skidmore, A., "Imaging Spectrometry and vegetation science", Img Spec 4(1), 978-0-306-47578-8 (2002)

[2] Ge, Y. Atefi, A. Zhang, Miao, C. Ramamurthy, RK. Sigmon, B. Yang, J. Schnable, JC. "High-throughput analysis of leaf physiological and chemical traits with VIS-NIR-SWIR spectroscopy: a case study with a maize diversity panel.", Plant Methods 15, (2019)

[3] Wang, S. Gian, K. Wang, Z. Ainsworth, E. Zheng, T. Townsend, P. Li, K. Moller, C. Wu, G. Jiang, C. "Unique contributions of chlorophyll and nitrogen to predict crop photosynthetic capacity from leaf spectroscopy", Journal Exp Bot 72, (2021)

[4] Yendrek, C.R., Tomaz, T., Montes, C.M., Cao, Y., Morse, A.M., Brown, P.J., McIntyre, L.M., Leakey, A.D., and Ainsworth, E.A. "High-throughput phenotyping of maize leaf physiological and biochemical traits using hyperspectral reflectance", Plant Physiol 173, (2017)

[5] Cotrozzi, L., Peron, R., Tuinstra, M.R., Mickelbart, M.V., and Couture, J.J. "Spectral phenotyping of physiological and anatomical leaf traits related with maize water status", Plant Physiol 184, (2020)

[6] Grzybowski, M. Wijewardane, N. Atefi, A. Ge, Y. Schnable, JC. "Hyperspectral reflectance-based phenotyping for quantitative genetics in crops: Progress and challenges", Plant Comms, (2021)

[7] Tucker, TC. "Diagnosis of Nitrogen Deficiency in Plants", Nitrogen in Crop Production 16(249 – 255), (1984)

[8] Wang, J. Jin, J. Song, Z. Wang, J. Zhang, L. Rehman, T. Ma, D. Carpenter, N. Tuinstra, M. "LeafSpec: An accurate and portable hyperspectral corn leaf imager", Comp and Elec in Ag 169, (2019)

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