



Prediction of Flavonoids in Maize Under Different Nitrogen Inputs by Hyperspectral Sensing and Machine Learning

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Abstract

This study aimed to accuracy of predicting flavonoids in maize plants subjected to different nitrogen rates using hyperspectral reflectance and machine learning (ML) algorithms. The experiment was carried out in randomized blocks in a 4 x 5 factorial design (four N inputs: 0; 30; 60 and 120% of the recommended N input; and five readings of the reflectance spectra in maize leaves from different vegetative stages: V6, V8, V10, V12 and V14, in four replications. N inputs were applied in the V4 and V8 phenological stages, using urea as the N source. For hyperspectral analysis, four leaves from each treatment were collected and analyzed using a spectroradiometer, capturing the spectrum in the 350 to 2500 nm range. Subsequently, the leaf samples used in the reflectance readings were dried and analyzed by ultra-performance liquid chromatography in three repetitions, quantifying daidzein 1 (D1), daidzein 2 (D2), genistein 1 (G1) and genistein 2 (G2). Data obtained was subjected to machine learning analysis, testing two data set input configurations: wavelengths (WL) and calculated spectral bands, and D1, D2, G1, G2 and total isoflavones as output variables. The ML algorithms tested were artificial neural networks, REPTree, M5P decision tree, ZeroR, Random Forest and support vector machine (SVM), evaluated according to their performance by the correlation coefficient and mean absolute error. The results show that the SVM algorithm had the highest accuracy in predicting the variables D1, D2, G1, G2 and total isoflavones, outperforming the other algorithms when WL was used as input in dataset.

Keywords: computational intelligence, isoflavones, secondary metabolites, spectroradiometry, support vector machine