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Prediction of adulteration level in bulk rice by modeling LIBS data using an extreme gradient boosting classifier

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Rice is the staple food widely consumed by more than half of the world's population. This cereal has a remarkable nutritional value since it contains minerals, vitamins, fibers, and essential amino acids which are necessary to build muscles and to maintain proper cellular functions[1]. Fraudulent labeling and adulteration are the main concerns in the pady industry due to the huge demand for rice products in the global market. Rice authenticity evaluation has therefore become in a quality requirement for protecting interests of consumers, traders and other stakeholders[2]. Laser induced breakdown spectroscopy (LIBS) is an interesting analytical technique for food authentication purposes, since it is capable of quickly providing spectra which are true fingerprints of sample elemental composition, requiring minimal sample preparation. In the present work, LIBS spectra obtained from rice analysis were assisted by Uniform Manifold Approximation and Projection for Dimension Reduction (UMAP) and Extreme Gradient Boosting (XGBoost) for predicting adulteration level in bulk rice samples. A total of 150 bulk rice samples purchased from local markets were individually ground using a cryogenic mill and converted into pellets by the application of 10 tons of pressure. Then, two pellets per samples were analyzed by LIBS spreading forty laser pulses on each pellet in different locations, resulting in 80 spectra per rice sample. The analyzed samples comprised 32 rice samples from pure Indica variety (high-quality) plus 118 samples adulterated at 10, 20, 30, and 40% with the Japonica variety (inferior-quality). The obtained spectra were preprocessed using Microsoft Excel® (2016) for base line correction and peak height determination. Next, UMAP was carried out to detect sample grouping trends and an XGBoost classifier was applied for selecting input variables and distinguishing among pure and adulterated rice samples, as well as identifying their level of adulteration. Fig. 1 shows average spectra obtained from pure and adulterated samples. The pattern distribution of rice samples is represented by Fig. 2, where a notable separation between the classes studied can be observed, mainly for the variety of pure rice.

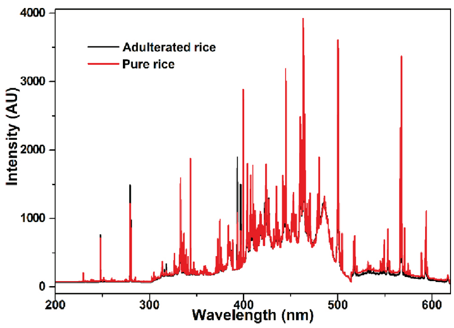

Figura 1.
Average spectra of pure and adulterated rice samples.

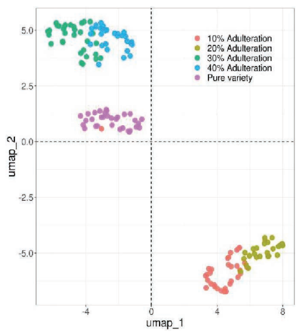

Figura 2.
Score plot of the spectral variables.

The modeling was evaluated by five-fold cross-validation and its performance was measured by calculating the overall accuracy as the ratio between all correct predictions and total number of examined cases. The spectral data size was reduced by choosing emission lines according to its importance for classification, which favored computing management to create a suitable model. The optimized parameter values were mtry = 14, trees = 589, min_n = 9, tree_depth = 12, learn_rate = 2.3×10^{-7}, loss_reduction = 2.7×10^{-4}, and sample_size = 0.997. Finally, the identification of rice adulteration level was accomplished with an accuracy of 97% in the test step, indicating a high success rate to distinguish pure and adulterated rice samples. The proposed method proved the potential of the LIBS technique for detecting adulterations in bulk rice samples with remarkable analytical features including simple, fast, low-cost, safe, and reliable measurements, based on sample mineral composition.

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