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Principal Component Analysis Combined Machine Learning Techniques on Pharmaceutical Samples by Laser Induced Breakdown Spectroscopy

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Abstract : Laser-induced breakdown spectroscopy (LIBS) is a rapid optical atomic emission spectroscopy which is used for material identification and analysis with the advantages of in-situ analysis, elimination of intensive sample preparation, and micro-destructive properties for the material to be tested. LIBS delivers short pulses of laser beams onto the material in order to create plasma by excitation of the material to a certain threshold. The plasma characteristics, which consist of wavelength value and intensity amplitude, depends on the material and the experiment's environment. In the present work, medicine samples' spectrum profiles were obtained via LIBS. Medicine samples' datasets include two different concentrations for both paracetamol based medicines, namely Aferin and Parafon. The spectrum data of the samples were preprocessed via filling outliers based on quartiles, smoothing spectra to eliminate noise and normalizing both wavelength and intensity axis. Statistical information was obtained and principal component analysis (PCA) was incorporated to both the preprocessed and raw datasets. The machine learning models were set based on two different train-test splits, which were 70% training – 30% test and 80% training – 20% test. Cross-validation was preferred to protect the models against overfitting; thus the sample amount is small. The machine learning results of preprocessed and raw datasets were subjected to comparison for both splits. This is the first time that all supervised machine learning classification algorithms; consisting of Decision Trees, Discriminant, naïve Bayes, Support Vector Machines (SVM), k-NN(k-Nearest Neighbor) Ensemble Learning and Neural Network algorithms; were incorporated to LIBS data of paracetamol based pharmaceutical samples, and their different concentrations on preprocessed and raw dataset in order to observe the effect of preprocessing.

Keywords : machine learning, laser-induced breakdown spectroscopy, medicines, principal component analysis, preprocessing
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