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Comprehensive Machine Learning-Based Glucose Sensing from Near-Infrared Spectra

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Abstract : Context: This scientific paper focuses on the use of near-infrared (NIR) spectroscopy to determine glucose concentration in aqueous solutions accurately and rapidly. The study compares six different machine learning methods for predicting glucose concentration and also explores the development of a deep learning model for classifying NIR spectra. The objective is to optimize the detection model and improve the accuracy of glucose prediction. This research is important because it provides a comprehensive analysis of various machine-learning techniques for estimating aqueous glucose concentrations. Research Aim: The aim of this study is to compare and evaluate different machine-learning methods for predicting glucose concentration from NIR spectra. Additionally, the study aims to develop and assess a deep-learning model for classifying NIR spectra. Methodology: The research methodology involves the use of machine learning and deep learning techniques. Six machine learning regression models, including support vector machine regression, partial least squares regression, extra tree regression, random forest regression, extreme gradient boosting, and principal component analysis-neural network, are employed to predict glucose concentration. The NIR spectra data is randomly divided into train and test sets, and the process is repeated ten times to increase generalization ability. In addition, a convolutional neural network is developed for classifying NIR spectra. Findings: The study reveals that the SVMR, ETR, and PCA-NN models exhibit excellent performance in predicting glucose concentration, with correlation coefficients (R) > 0.99 and determination coefficients (R^2)> 0.985. The deep learning model achieves high macro-averaging scores for precision, recall, and F1-measure. These findings demonstrate the effectiveness of machine learning and deep learning methods in optimizing the detection model and improving glucose prediction accuracy. Theoretical Importance: This research contributes to the field by providing a comprehensive analysis of various machine-learning techniques for estimating glucose concentrations from NIR spectra. It also explores the use of deep learning for the classification of indistinguishable NIR spectra. The findings highlight the potential of machine learning and deep learning in enhancing the prediction accuracy of glucose-relevant features. Data Collection and Analysis Procedures: The NIR spectra and corresponding references for glucose concentration are measured in increments of 20 mg/dl. The data is randomly divided into train and test sets, and the models are evaluated using regression analysis and classification metrics. The performance of each model is assessed based on correlation coefficients, determination coefficients, precision, recall, and F1-measure. Question Addressed: The study addresses the question of whether machine learning and deep learning methods can optimize the detection model and improve the accuracy of glucose prediction from NIR spectra. Conclusion: The research demonstrates that machine learning and deep learning methods can effectively predict glucose concentration from NIR spectra. The SVMR, ETR, and PCA-NN models exhibit superior performance, while the deep learning model achieves high classification scores. These findings suggest that machine learning and deep learning techniques can be used to improve the prediction accuracy of glucose-relevant features. Further research is needed to explore their clinical utility in analyzing complex matrices, such as blood glucose levels.

Keywords : machine learning, signal processing, near-infrared spectroscopy, support vector machine, neural network
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