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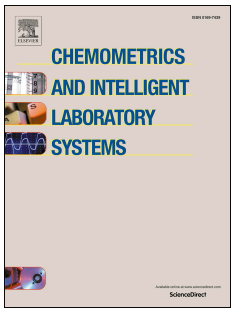

Modern practical convolutional neural networks for multivariate regression: Applications to NIR calibration

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Modern practical convolutional neural networks for multivariate regression: applications to NIR calibration

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Abstract

In this study, we investigate the use of convolutional neural networks (CNN) for near infrared (NIR) calibration. We propose a unified CNN structure that can be used for general multivariate regression purpose. The comparison between the CNN method and the partial least squares regression (PLSR) method was done on three different NIR datasets of spectra and lab reference values. Datasets are from different sources and contain 6998, 1000 and 415 training and 618, 597 and 108 validation samples, respectively. Results indicated that compared to the PLSR models, the CNN models are more accurate and less noisy. The convolutional layer in the CNN model can automatically find the suitable spectral preprocessing filter on the dataset, which significantly saves efforts in training the model.

Keywords: Near-infrared spectroscopy; Multivariate regression; Partial least squares regression; Convolutional neural networks; Automatic spectral preprocessing

1 Introduction

Convolutional neural networks have recently become the popular solution for different machine learning tasks, including object detection [1], image classification [2], natural language processing [3], time series classification [4] and many other applications.

Implementation of neural networks (NN) as a chemometrics technique is relatively recent. Previous researches have shown that artificial neural networks (ANN) can be used as a tool for data reduction, pattern recognition and multivariate regression in spectroscopic analysis [5] [6] [7] [8] [9]. Comparison of ANN to the PLS regression has been done on various spectroscopic datasets [10]. We have also proposed some replacement methods for solving nonlinearity in multivariate regression, such as Gaussian process regression [11] and Bayesian graphical modeling [12]. Common features of these methods are high in flexibility and adaptability, but difficult to train and prone to overfitting.

Considering a lot of recent contributions to the neural networks improvements, there is very little advances on their application to the resolution of chemometrics tasks. Especially, there are few examples on implementation of CNN for spectroscopic analysis. Two very recent works