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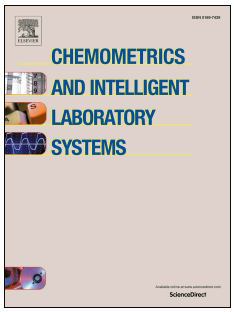

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A Selective Review and Comparison for Interval Variable Selection in Spectroscopic Modeling

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Abstract

Dimension reduction and variable selection are two types of effective methods that deal with high-dimensional data. In particular, variable selection techniques are of wide-spread use and essentially consist of individual selection methods and interval selection methods. Given the fact that the vibrational spectra have continuous features of spectral bands, interval selection instead of individual spectral wavelength point selection allows for more stable models and easier interpretation. Numerous methods have been suggested for interval selection recently. Therefore, this paper is devoted to a selective review on interval selection methods with partial least squares (PLS) as the calibration model. We described the algorithms in the five classes: classic methods, penalty-based, sampling-based, correlation-based, and projection-based methods. Finally, we compared and discussed the performances of a subset of these methods on three real-world spectroscopic datasets.

Keywords

Spectroscopy; PLS; interval variable selection

1. Introduction

In recent years, the extensive use of multivariate calibration methods in multi-component spectral analysis has made them extremely popular techniques, especially for vibrational spectral

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