

**Application of Two Novel Partial Least Squares-Based Regression Methods to the Analysis of
Spectral Datasets**

by

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Abstract

This work introduces two novel algorithms for multivariate regression: a partial least squares (PLS) variable selection method based on resampling and a PLS method using data transformation of the PLS weights (twPLS). The algorithms are tested on three spectral datasets (near-infrared and Raman) by predicting univariate response variables. The results are compared with the predictions of three other established methods comprising standard PLS, variable selection by sparse PLS (SPLS) and variable selection by variable importance in projection (VIP). Compared with the standard PLS method, the novel algorithms clearly improve predictions for one dataset and show slightly more accurate predictions for two other datasets.

The two novel algorithms show comparable results with the SPLS and variable selection by VIP for all three datasets. These results demonstrate the effectiveness of the new approaches.