Non-linear calibration models for near infrared spectroscopy

Different calibration techniques are available for spectroscopic applications that show nonlinear behavior. This comprehensive comparative study presents a comparison of different nonlinear calibration techniques: kernel PLS (KPLS), support vector machines (SVM), least-squares SVM (LS-SVM), relevance vector machines (RVM), Gaussian process regression (GPR), artificial neural network (ANN), and Bayesian ANN (BANN). In this comparison, partial least squares (PLS) regression is used as a linear benchmark, while the relationship of the methods is considered in terms of traditional calibration by ridge regression (RR). The performance of the different methods is demonstrated by their practical applications using three real-life near infrared (NIR) data sets. Different aspects of the various approaches including computational time, model interpretability, potential over-fitting using the non-linear models on linear problems, robustness to small or medium sample sets, and robustness to pre-processing, are discussed. The results suggest that GPR and BANN are powerful and promising methods for handling linear as well as nonlinear systems, even when the data sets are moderately small. The LS-SVM is also attractive due to its good predictive performance for both linear and nonlinear calibrations.

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