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J-Score: a new joint parameter for PLSR model performance evaluation of spectroscopic data

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Introduction

Partial Least Squares Regression (PLSR) is a widely used algorithm in multivariate data analysis, especially in spectroscopic measurements. Various parameters have been proposed to evaluate PLSR model performance [1], but selecting the optimal number of Latent Variables (LVs) and the best preprocessing technique can be challenging for non-experienced analysts. This study introduces a new parameter, the J-Score, which combines multiple model evaluation parameters into a single indicator [2].

Aim of study

- Introduce a single indicator that combines multiple regression model evaluation parameters, describing different properties of the model.
- To provide an automated and objective way to assess PLSR models and facilitate decision-making for analysts.
- Assist in selecting the appropriate number of LVs and optimal preprocessing techniques.

Materials and Methods

The J-Score is calculated by combining three model evaluation parameters: the Inverse Ratio of Performance to Deviation (RPD), the Calibration to Validation Error ratio and the Regression Vector Noise Index.. These parameters are transformed into numerical indexes that range from 0 to 1 (0 being optimal) and then averaged to obtain the J-Score.

$$\text{J-Score} = \left(\frac{\text{RMSE}_{CV}}{s_Y} + 1 - \frac{\text{RMSE}_{Cal}}{\text{RMSE}_{CV}} + \text{NI}_{RV}\right)/3$$

The study uses three spectroscopic datasets with different characteristics to evaluate the behavior of the J-Score in different scenarios:

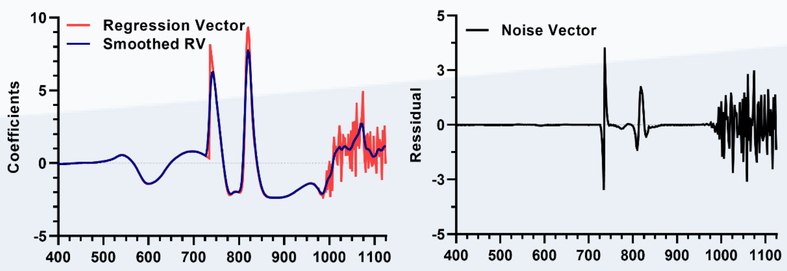
- Dataset 1: Raman spectra of meat to predict Iodine Value. (Lyndgaard *et al*., *J Raman Spectrosc*, 2012)
- Dataset 2: NIR spectra of wine fermentation to predict pH and density. (Cavaglia *et al*., *Food Control*, 2020)
- Dataset 3: FTIR spectra of forages to predict humidity. (Ruisánchez *et al*. *Chemometr Intell Lab Syst*, 2002)

Results

Regression Vector noise quantification

The regression vector noise index measures the noise [3] in the regression vector of a PLSR model, which is a diagnostic tool to evaluate if it is overfitted to the calibration data.

1. Smoothing the regression vector (with an automated algorithm).
2. Calculating the residual between the original and smoothed vectors.
3. Adding up all the absolute residuals.
4. Normalizing the result by the summatory of the absolute values of the original RV.

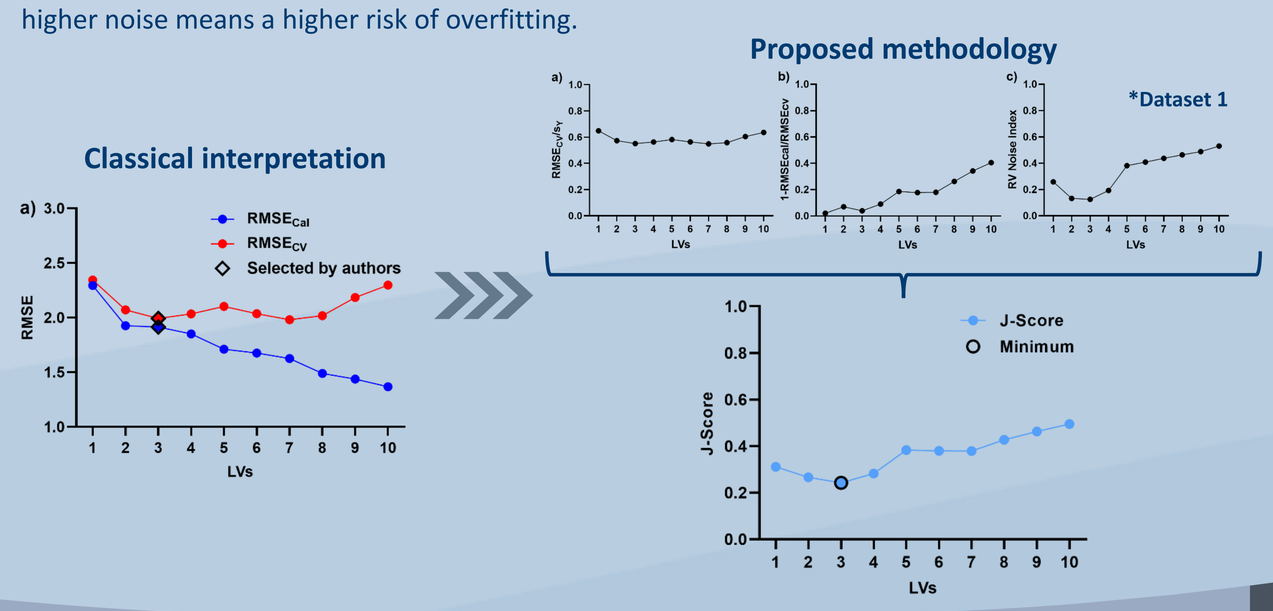


$$NI_{RV} = \frac{\sum|RV - RV_{smoothed}|}{\sum|RV|}$$

J-Score: a joint index

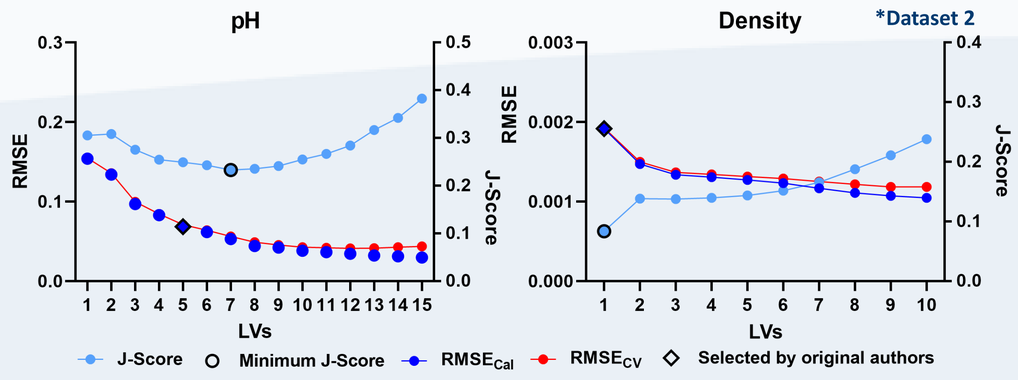
The J-Score is composed of several indices that provide a comprehensive evaluation of the performance and reliability of a Partial Least Squares Regression (PLSR) model.

- **Inverse RPD:** This index measures how well the calibration data is explained by the model.
- **Calibration to Validation Error Ratio**: This index measures the predictive ability of the model.
- **Regression Vector Noise Index**: This index quantifies the degree of overfitting in the model. A higher noise means a higher risk of overfitting.



Selection of the model dimensionality

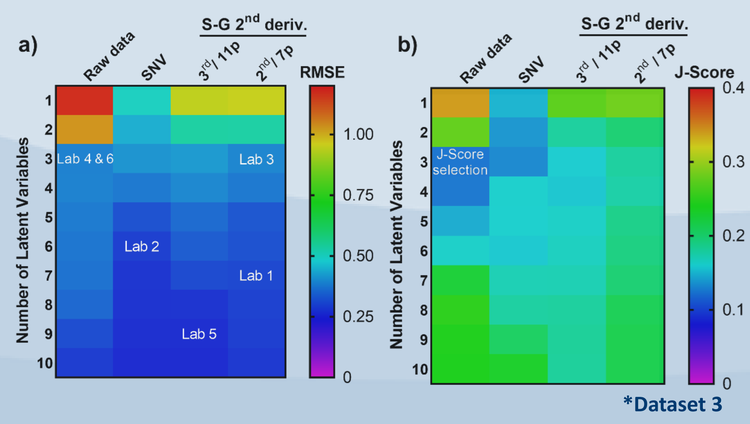
The J-Score aids in selecting the optimal number of latent variables for the model, providing a clearer minimum and helps analysts make objective and parsimonious decisions in model evaluation.



The J-Score provides a comprehensive assessment of the PLSR model's performance, including predictive ability, overfitting, noise level and the fit of the model.

Selection of the optimal preprocessing

When applying preprocessing techniques to spectroscopic data, various transformations, scaling methods, and noise reduction approaches can be used. Each preprocessing method may have different effects on the model performance.



By using the J-Score, as opposed to using the $RMSE_{CV}$, there is a clear selection of the optimal preprocessing method and model dimensionality. This can help the analyst to objectively assess the impact of different preprocessing methods and make an informed decision.

Conclusions

- The J-Score provides a more objective and consistent method for selecting the optimal number of LVs compared to other evaluation metrics, such as RPD, $RMSE_{CV}$ or $RMSE_P$.
- The J-Score is effective for different types of spectroscopic data, including UV-Vis, Raman, MIR, and NIR spectra.
- The J-Score offers an objective and global way of comparing models, reducing the bias introduced by subjective evaluation and individual expertise.

The J-Score, which combines multiple indices related to model performance, is an effective tool for selecting the optimal dimensionality and preprocessing method for Partial Least Squares Regression (PLSR) models.

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