In the field of chemometrics, an important issue in multivariate calibration is model updating. Model updating is the adaption process in which a model obtained for a given set of samples and measurement conditions (primary) is updated to predict the analyte in new samples and measurement conditions (secondary). The calibration method partial least squares is applied with two new updating approaches. In one approach, only one updated model is obtained to predict the analyte amount in both primary and secondary conditions. The other approach forms two updated models in which one model is used to predict in primary conditions and second model is used to predict in secondary conditions. Both approaches are evaluated with near-infrared spectral datasets. Datasets include spectra of soil, corn, olive oil adulterated with sunflower and pharmaceutical tablets. Fusion process and single merits are used to select models. Model selection methods are evaluated based on prediction errors using selected models.

**Objective**

- Develop a new effective modal updating approach.

**Model Updating Approach**

**1b-PLS**: 1 updating model

\[
\begin{align*}
\mathbf{y} &= \mathbf{Xb} \\
\mathbf{b} &= \mathbf{X}^{-1}\mathbf{y} \\
\end{align*}
\]

**2b-PLS**: 2 updating models

\[
\begin{align*}
\mathbf{y} &= \mathbf{Xb} \\
\mathbf{b} &= \mathbf{X}^{-1}\mathbf{y} \\
\end{align*}
\]

**Data Centering**

- Local mean centering:
  - \(x\) and \(y\) are centered across samples to respective means.
  - Mean of \(x\) and \(y\) are used to center validation samples in secondary condition.

**Model Measures**

- **Bias**:
  - Primary Calibration (P)
  - Secondary Calibration (S)
  - Secondary Validation (V)
  - Bias Mean Square Error (BMSE)
    \[ \text{BMSE} = \sum_{i=1}^{N} \left( \mathbf{y}_i - \hat{\mathbf{y}}_i \right)^2 \]
  - Root Mean Square Error (RMSE)
    \[ \text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \mathbf{y}_i - \hat{\mathbf{y}}_i \right)^2} \]

**Conclusion**

- The model selection method is evaluated with the following datasets:
  - Soil (50 wavelengths)
  - Corn (50 wavelengths)
  - Pharmaceutical tablets (400 wavelengths)

- The model selection method is applied to the following datasets:
  - Soil (50 wavelengths)
  - Corn (50 wavelengths)
  - Pharmaceutical tablets (400 wavelengths)

- The model selection method is evaluated for the following cases:
  - Primary Calibration (PC)
  - Secondary Calibration (SC)
  - Primary Validation (PV)
  - Secondary Validation (SV)

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