Calibration transfer between different types of multisensor systems

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Multisensor systems, also known as “electronic tongues”, are promising analytical tools for express analysis of various complex parameters in liquids, like e.g. taste, toxicity, etc. These systems are a combination of hardware and software parts. Hardware part consists of chemical sensor array and devices for sensor response registration. Two most commonly used sensor types are potentiometric and voltammetric. Software part is related to chemometric techniques. Typically multivariate regression modelling is employed to relate the response of sensor system with parameter of interest. A good model requires considerable efforts and large number of samples, which can be unique, expensive and hard to get. It would be very practical to have a method capable of multivariate calibration transfer between various multisensor systems working on different principles.

In our previous research a simple algorithm based on PCA decomposition has been suggested for calibration transfer between different analytical methods. It can convert the data from one instrumental format to another [1]. In this study we apply the proposed strategy to transfer calibration models between voltammetric and potentiometric multisensor systems. Sample set consisted of 8 types of grape musts. All the samples were measured at least three times with two sensor arrays: voltammetric of 4 sensors with metal oxide modified surface operated in cyclic voltammetry mode, and potentiometric of 26 plasticized polymeric membrane sensors. Cyclic voltammograms were compressed by kernel method, 10 kernels for each sensor were used. Resulting voltammetric (VA) data were 8×40 matrix, while potentiometric one was 8×26. The VA data were used to build PLS regression models to predict total acidity, potassium concentration, tartaric acid concentration and other parameters of grape must. RMSEP values of these models

for total acidity were around 0.08 (for the range 0.66-0.96 lg C(TA)). Potentiometric data were converted into voltammetric response shapes with suggested algorithm and were used further to predict the same parameters. Corresponding RMSEP for TA was 0.05 (this decrease can be attributed to the higher sensitivity of potentiometric sensors towards TA which is confirmed by RMSEP values of the original potentiometric model equal 0.02). Similar results were obtained for several other parameters.

These results show that data conversion between different sensor arrays based on different working principles is possible and this fact can be employed for building cross-platform multivariate regression models.

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References

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