Genetic Multivariate Calibration Method for Complex Analytical Data

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Quantitative molecular spectroscopic techniques in analytical chemistry have been evolved into quite highly sophisticated tools with the help of chemometrics and modern computer technology. Spectroscopic analysis offers tremendous advantages over conventional wet chemical methods and separation based chromatographic techniques. They are much faster and consume less hazardous chemicals which results in much cheaper analysis. On the other hand, real life samples contain several components and the spectra of these mixtures suffer from several overlapping peaks. Therefore, univariate methods are not able to generate calibration models in order to determine quantitatively the components of the mixtures.

Multivariate calibration makes it possible to use instrument responses at several wavelengths and provides significant improvement in the modeling of concentration information. A number of different multivariate calibration methods have been developed in the past and some of them have been incorporated into commercial software packages such as principal component regression (PCR) and partial least squares (PLS) which are based on principal component analysis (PCA) [1-2]. Classical least squares (CLS) and inverse least squares (ILS) are the other two well known methods that relies on multiple linear regression and much simpler in terms of the mathematics involved in the model building step. All the methods mentioned above use the full spectrum information to generate multivariate calibration methods. Quite often the information contained in a given spectrum may not be all linear with the component concentrations and may even contain noise. In cases like these may require some wavelength selection in order to improve the quality of the calibration models.

Genetic Algorithms (GA) are global search and optimization methods based upon the principles of natural evolution and selection as developed by Darwin. GA’s based methods are well suited for such complex variable selection problems and various publications have been reported in recent years [3]. We have developed a number of genetic algorithm based calibration methods such as genetic inverse least squares (GILS) and genetic partial least squares (GPLS) [4-5]. Several applications of these methods to infrared and fluorescence spectroscopy have been demonstrated and compared with the conventional multivariate calibration methods. The results were shown that GA based methods improves the prediction ability of multivariate calibration by selecting the most concentration related wavelengths and eliminating the unnecessary information.

References