Discrimination Analysis of Gallstones by Near Infrared Spectrometry Using a Soft Independent Modeling of Class Analogy

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A method to discriminate human gallstones by near infrared(NIR) spectrometry using a soft independent modeling of class analogy (SIMCA) has been studied. The fifty NIR spectra of gallstones in the wavenumber range from 4500 to 10,000 cm^{-1} were measured. The forty samples were classified to three classes, cholesterol stone, calcium bilirubinate stone and calcium carbonate stone according to the contents of major components in each gallstone. The training set which contained objects of the different known class was constructed using forty NIR spectra and the test set was made with ten different gallstone spectra. The number of important principal components(PCs) to describe the class was determined by cross validation in order to improve the decision criterion of the SIMCA for the training set. The score plots of the class training set whose objects belong to the other classes were inspected. The critical distance of each class was computed using both the Euclidean distance and the Mahalanobis distance at a proper level of significance(α). Two methods were compared with respect to classification and their robustness towards the number of PCs selected to describe different classes.