Chemometric methods for identification and classification of microorganisms by micro-Raman spectroscopy

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Fast identification of microorganism is fundamental not only in hospitals, but also in laboratories. For this purpose several techniques and methods were suggested, whereas Raman spectroscopy is one of the most interesting [1]. Micro-Raman spectroscopy is a fast and sensitive method which requires only a minimal sample preparation and in addition a minimal amount of sample volume. It is shown that Raman spectroscopy is capable of differentiation of pathogenes [2]. This method is useful even for clean-room-relevant biological contaminations [3]. For the identification of microorganisms modern chemometric techniques are required.

In our contribution different chemometric methods, e.g. artificial neural networks, linear discriminant analysis and support vector machines, will be evaluated regarding their capabilities for identification of microorganisms. The primary points of the investigation are the optimization algorithms for improving the abilities of bacterial classifiers and to minimize the error at the identification process. Among the optimization algorithms are methods which handle classifiers depending on parameters and schemas for combining classifiers to gain the accuracy of the output.

Furthermore, several techniques are presented to expand the capabilties of the classifiers with emphasis on novelty detection and meta information. The presented techniques combines classifiers to a problem adopted hierarchical approach and the one-against-the-rest schema.

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