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Exploratory Analysis Strategies for High Dimensional Mid-Infrared Microspectroscopy Data from Tissue Sections

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Mid-infrared micro-spectroscopy is being increasingly relied upon to survey tissue biopsy samples in order to determine the distribution of chemical species, distinguish different tissue domains as well as to detect and distinguish tissue pathologies. Micro-spectroscopic mapping or imaging of tissue sections result in a large set of spectra that are spatially resolved over the sample. Analysis of each spectrum in the set of spectra represents an onerous task while visual assessment of the raw individual images generally provides little or no information of histological relevance. Clearly, some form of automated analysis that compactly represents the chemical information of the sample is desirable. The analysis of spectroscopic images or maps should preserve the spatial information of the sample as well as highlight specific chemical information and histological features.

In some cases, one has a priori knowledge of the class spectra or chemical constituents of the sample. The spatial distribution of these constituents in the sample can be determined by matching sample spectra to reference spectra of the constituents. Linear discriminant analysis has been used in this fashion to classify sample tissue spectra based on their similarity to reference spectra used in the training set to determine discriminant function. When the target disease or condition is known to produce a distinct spectral feature or pattern, a similar confirmatory analysis technique or pattern matching method can be used. Generally, little is known about the tissue constituents or the spatial distribution of these constituents. In the majority of cases, the spectroscopic image or map needs to be explored to determine the distinguishing characteristics of the sample.

In this presentation, of a number of exploratory data analytic methods will be discussed. For example, simple functional group mapping, principal component analysis (PCA) and cluster analysis (CA) are common exploratory analysis techniques that have been used to analyze spectroscopic images and maps of tissues. The strengths and weakness various pre-processing and processing strategies for PCA and CA of micro-spectroscopy FTIR-imaging of tissue sample are discussed. Novel approaches will be introduced that combine morphological segmentation with spectroscopic characterization. These approaches can simultaneously exploit the histological and spectroscopic information available from the sample or alternatively find commonalities between the histology of the sample and the spectroscopy of the sample in an unsupervised and automated fashion.

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