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## Preprocessing and exploratory analysis of Surface-Enhanced Raman Scattering (SERS) data for diagnosis with immunoassays

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Surface-Enhanced Raman Scattering (SERS) has been used as an analytical technique that reaches low detection limits for a fast diagnosis of diseases (1), and this can be enhanced if the SERS spectra are analyzed with pattern recognition methods based on machine learning. However, the large number of SERS spectra required to classify highly variable biological samples demands preprocessing strategies for the input in the machine learning algorithms. This work presents the methods to preprocess and explore SERS data acquired from a magnetic immunoassay for detecting human IgM antibodies with nanoprobe fabricated with gold nanoparticles and Nile Blue (Raman reporter). The dataset comprises 60 SERS data equally distributed in 10 human antibody type IgM (antigen) concentrations, viz. 0, 10, 30, 60, 80, 100, 250, 500, 750 and 1000 ng/mL. The SERS data have cubic format, i.e. in each one of the 21 x 21 immunoassay positions (x, y) spaced by 2  $\mu\text{m}$  there is a spectrum with 1021 points ranging from 99 to 898  $\text{cm}^{-1}$  Raman shift. The SERS data were represented in a format with 26460 rows (instances) and 1026 columns (features and classes). The exploratory analysis and preprocessing of the spectra were performed in an iterative way. Statistics metrics, data visualization and similarity measures. (2) were used to detect outliers, reduce background noise (3) and determine the spectral regions with the most significant peaks for distinguishability. (2) Four outlier spectra were identified, one of which had an unexpected spike at the Raman reporter band (592  $\text{cm}^{-1}$ ) and the others had a wide region with 0 intensity. The outliers were removed from the dataset, and a region extending  $\pm 100 \text{ cm}^{-1}$  around the Raman reporter band was selected. The background noise was removed by applying polynomial fitting (degree = 5). Only the spectra with peak at the Raman reporter band were selected. The distance measures between spectra intensities (a.u) for all classes were, in average, about 172k (min. 116k, max. 272k). The preprocessing methods and the exploratory analysis applied to the SERS data will allow for applying pattern recognition methods with machine learning for diagnosis with immunoassays.

**Palavras-chave:** Preprocessing. Exploratory analysis. SERS.

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