

Using AI for fast treatment of multiple Raman spectra

Trabalho #13

Apresentação Oral

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The analysis and comparison of Raman spectra can be use to demonstrate different structures on crystals, identify active pharmaceutical ingredients and its forms on medicines, or measure the presence and quantity of nutrients on organic compounds. However, in order to compare and analyse different Raman spectra a series of procedures should be followed, such as removing spikes and background, normalizing data and performing average of multiple acquisitions, that are normally done by hand.

While the power of Raman spectra analysis can be greatly increased by the introduction of machine learning algorithms, such algorithms usually require several data for computer training. And since one Raman spectra contains a huge number of points, which consist on a huge dimension for the input data of the machine learning algorithm, the complexity of this algorithm should be really high in order to make good predictions, which consist on a high number of free parameters. Thus, machine learning algorithms for Raman spectra analysis requires a huge amount of spectra as input for training, and manually treating them became an impossible task.

In this work, it will be present some computer algorithms that can be useful in order to automatically pretreat and process Raman spectra data for further analysis.

Comentários adicionais

É um trabalho simples porém bastante relevante, dado que ainda são poucas pesquisas que utilizam machine learning na física e menos ainda para análise de espectro Raman. Temos dois artigos em fase de preparação sobre o assunto, um sobre como melhorar a resposta final do machine learning e outro sobre como tratar os dados, ambos com espectro Raman e ambos com objetivos específicos e dados reais, em áreas diferentes.