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Pre-processing Raman data via deep learning method

Raman spectroscopy is a type of analytical technique that uses the interaction of light with a sample to provide information about its atomic and molecular properties. However, Raman spectra are frequently overshadowed by inconsistencies in baselines and various sources of noise. These defects and contributions to the Raman data must be rectified before identifying or categorizing the samples. Accordingly, Raman data is processed using AI-based algorithms. To that end, we suggested the use of a deep learning approach as a pre-processing tool for Raman data. As a result, we tested two networks: the convolutional denoising autoencoder (CDAE) [1] and U-Net [2]. CDAE and U-Net networks were implemented to test two different pre-processing cases: denoising and denoising with baseline removal. In both cases, the superiority of the methods was evaluated using real and artificial Raman data. In the first case, we aimed to reconstruct high-quality (HQ) Raman spectra that included a background. Therefore, the networks were trained to map between noisy Raman data measured with different integration times, for example, 0.5 s as an input and HQ Raman data with 1 s as an output. As shown in Figure 1, the U-Net/CDAE network tries to estimate the HQ data in experiment data or predict the HQ artificial Raman data. Afterward, in the testing phase, the trained networks are used to predict the HQ data. In the second case, we aimed to reconstruct high-quality spectra with baseline removal. In other words, the aim of this case is to remove noise and background from the data at the same time. Therefore, the same noisy Raman data was used as an input, and the output was acquired by applying classical pre-processing methods (SG+SNIP on the HQ Raman data). Regarding the evaluation part in Figure 1, U-Net has the capability to remove the noise and baseline simultaneously, while the CDAE is only able to remove the noise. In conclusion, the suggested technique outperforms traditional methods in terms of time and error.

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