

Vector casting based spectra de-noising

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Spectral analysis involves processing of spectroscopic data patterns for quantification and/or identification of chemical or biological samples^[1]. However often the underlying data patterns consist of desired information about the sample obscured by noise and background or interferences of undesired signals. The differentiation between the noise and desired signal is challenging especially when the signal-to-noise-ratio (SNRs) is small. Thus to purify the ineluctable contamination of spectroscopic data with noise, it is imperative to apply post-processing techniques.

Existing noise reduction techniques such as the Savitzky - Golay filter (SG)^[2], smoothing based on the wavelet transform method^[3], the “perfect smoother” method^[4], and smoothing based on the “Wiener estimation”^[5], can reduce the noise level. However on the contrary they can also manipulate the desired signal.

Here, we propose a new method for the reduction of noise from spectra based on envelope detection followed by vector casting. As a first step we implemented an algorithm to detect the upper and lower envelopes of the noisy signal. This involves detection of available peaks of the signal. As a second step we casted vector lines from a starting already noise reduced point to subsequent not yet noise reduced data points. Then all vector lines that are confined within the envelopes were identified. The value of the data point, which is situated one increment right to the already noise reduced data point, is updated from the average slope of the selected vectors and the distance between the two neighboring data points. This whole casting and selection of new vector lines within a shifted new spectral window and averaging of intercepted vector lines is repeated as long as all raw data points have been replaced by noise reduced data points.

The developed method is relevant for the purification of spectroscopic signal having small signal-to-noise-ratio (SNR). Of course the technique cannot extract signal peaks with strength less than the noise level, however it can remove noise with minimized manipulation of characteristics of the desired signal as compared to the wavelet transform method and Savitzky-Golay method.

References

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