

Denoising Raman Spectra of Biological Samples Using Wavelets

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A range of applications of Raman spectroscopy in investigations of biological systems is emerging rapidly. The spectral analysis of these systems is difficult because of their complexity, and the noise superimposed on Raman signals.

Increasing the laser power and increasing the number of co-added scans are two standard methods to improve signal to noise (S/N) ratio. However, they are often counter productive. The former destroys the sample, and the latter changes sample properties because of drying.

In this work, we use wavelet transform to improve S/N ratio [1]. We apply different wavelet denoising methods [2] (fixed form threshold, SURE, Minimax, Penalize, Wavelet packet) to Raman spectra with different levels of S/N ratio, and analyze their efficiency. Two efficiency criterions were defined. One is the number of preserved vibrational bands in the denoised spectrum in comparison to the referent spectrum. The second criterion is the preservation of relative intensities of vibrational bands in the denoised spectrum. For this purpose, the series of Raman spectra was recorded from the same sample of rat skull bone. Different levels of S/N ratio in the recorded spectra were achieved by varying the number of scans and the laser power. The spectrum with the best S/N ratio was selected as the reference, and its vibrational bands were assigned using second derivatives. Spectra with smaller S/N ratios were denoised with wavelet transformations and their vibrational bands were assigned and compared with the reference. To check the first efficiency criterion we counted how many vibrational bands assigned to the referent spectrum were preserved in the denoised spectra. For second criterion the ratio of integral intensities of PO₄ and amid I band was compared between denoised and referent spectra. The efficiency of wavelet denoising was also tested for different wavelet families (Haar, Daubechies, Symlets, Coiflets, BiorSplines, ReverseBior, DMeyer), and compared with standard smoothing methods such as Block Averaging and Savitsky-Golay.

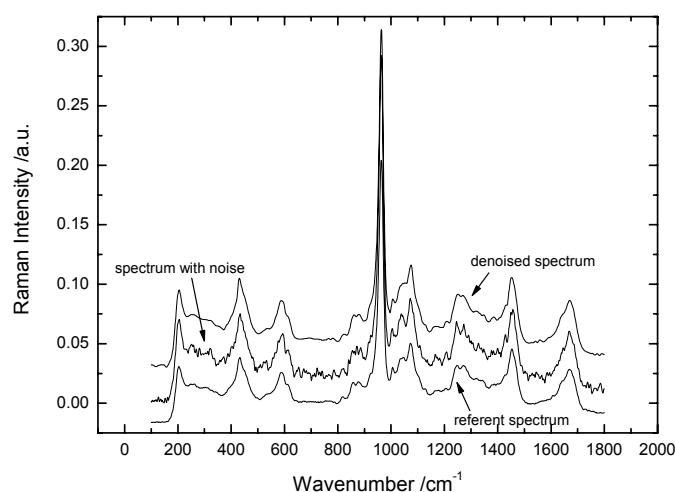


Fig. 1: Comparison of original, denoised and referent spectrum

- [1] C.R. Mittermayr, S.G. Nikolov, H. Hutter, M. Grasserbauer, *Chemometrics and intelligent laboratory systems* 34 (1996) 187-202
- [2] B.K. Alsberg, A.M. Woodward, M.K. Winson, J. Rowland, D.B. Kell, *The Analyst* 122 (1997) 645-652.