De-Noising ENMR Spectra by Wavelet Shrinkage

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Abstract

Wavelet Shrinkage de-noising is applied to Electrophoretic Nuclear Magnetic Resonance (ENMR) data. Both threshold rules for removing noise, namely soft and hard, proposed in Donoho's VisuShrink are used simultaneously. Soft thresholding is applied to fine levels of wavelet decomposition coefficients and hard thresholding to coarse levels. This implementation is coordinated by visualizing the features presented in ENMR spectra.

1: Introduction

Wavelet shrinkage (WS) has recently emerged as a powerful tool for extracting signals from noisy data [1]. While traditional linear methods of smoothing usually achieve noise suppression by broadening features significantly, WS is capable to entirely suppressing the noise as well as retaining features. Therefore it makes sense to apply WS to feature sensitive data such as high-resolution electrophoretic NMR (ENMR) data. ENMR is a method for resolving NMR spectra on the basis of electrophoretic mobilities of NMR active species [2]. Several practical factors such as magnetic gradients induced by currents in sample, resistive heating & convection, eletroosmosis, etc. result in obtaining noisy data. In this report, we present results of de-noising such ENMR data by WS.

2: Theory

2.1: The discrete wavelet transform

A discrete wavelet transform W is a linear operation which decomposes a signal f into a weighted sum of basis functions $\psi_{\nu,k}$

$$f(x) = \sum_{\nu} \sum_{k} c_{\nu,k} \psi_{\nu,k}(x) \qquad \nu, k \in Z. \tag{1}$$

The $\psi_{\nu,k}$ are generated from a single mother wavelet ψ by dilations and translations

$$\psi_{\nu,k}(x) = 2^{-\nu/2} \psi(2^{-\nu}(x-k)) \tag{2}$$

ere ν is the dilation scale index and k is the translation index. The empirical wavelet icients $c_{\nu,k}$ are obtained by projecting the signal f onto the wavelet basis set $\psi_{\nu,k}$ [3].

2.2: Wavelet shrinkage

Following Donoho and Johnstone [1][4][5], suppose a function f on $[0, 1]$ measured as noisy data

$$d_i = f(t_i) + \sigma z_i \quad i = 0, \ldots, n-1 \tag{3}$$

where $t_i = i/n$, $z_i \overset{iid}{\sim} N(0, 1)$ is a Gaussian white noise, and σ is a noise level.

In the wavelet space, (3) can be rewritten as

$$\begin{aligned} W(d_i) &= W(f(t_i) + \sigma z_i) \\ &= W(f(t_i)) + \sigma W(z_i) \end{aligned} \tag{4}$$

where $W(z_i) \overset{iid}{\sim} N(0, 1)$ is also a Gaussian white noise, if the basis functions are orthonormal.

Thus

$$f(t_i) = W^1(W(d_i) - \sigma W(z_i)). \tag{5}$$

In general $\sigma W(z_i) = w_i$ is unknown and can be estimated as λ_i. Two threshold rules, amely *soft* and *hard*, may be applied as:

$$\eta_S(w_i, \lambda_i) = \begin{cases} w_i - \lambda_i & w_i \geq \lambda_i \\ 0 & |w_i| < \lambda_i \\ w_i + \lambda_i & w_i \leq -\lambda_i \end{cases} \tag{6}$$

$$\eta_H(w_i, \lambda_i) = \begin{cases} w_i & |w_i| \geq \lambda_i \\ 0 & |w_i| < \lambda_i. \end{cases} \tag{7}$$

VisuShrink, λ_i is chosen as $\lambda_i = \sigma\sqrt{2logn}$. σ may be estimated by $m/.6745$ where m an absolute deviation of the wavelet coefficients at the finest level.

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hreshold choice generally produces 'noise-free' reconstruction [6], sometimes at nkage of genuine features. On the other hand, hard thresholding preserves peak heights) better, but can yield less smooth fits.
rink and combine both soft and hard threshold rules. The implementation

rval-adapted pyramidal filtering algorithm of Cohen, Daubechies, o the measured data $(d_i/\sqrt{n})$, obtaining empirical wavelet coef-

$og(n)\sigma/\sqrt{n}$, apply the soft thresholding coordinatewise to ents from the finest level up to a certain level ν_c; apply aining levels above ν_c.

ining the recovered data.

hough it appears to be two dimensional, we nce the experimental conditions such as trum is presented in Fig. 2. The ate periodically as functions of he implementation described

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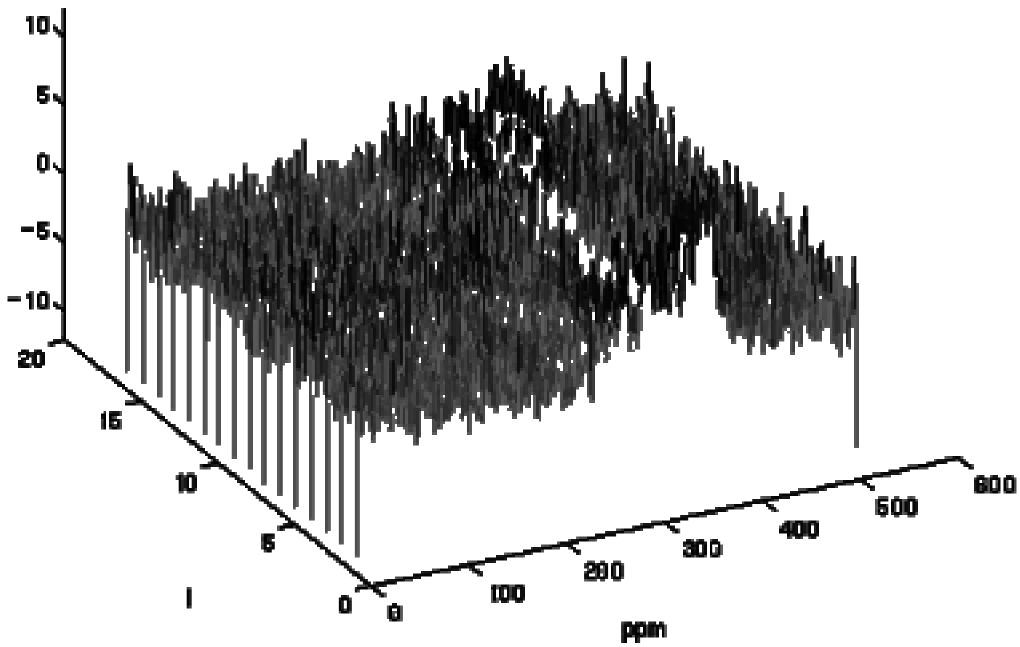

Figure 1. An ENMR spectrum.

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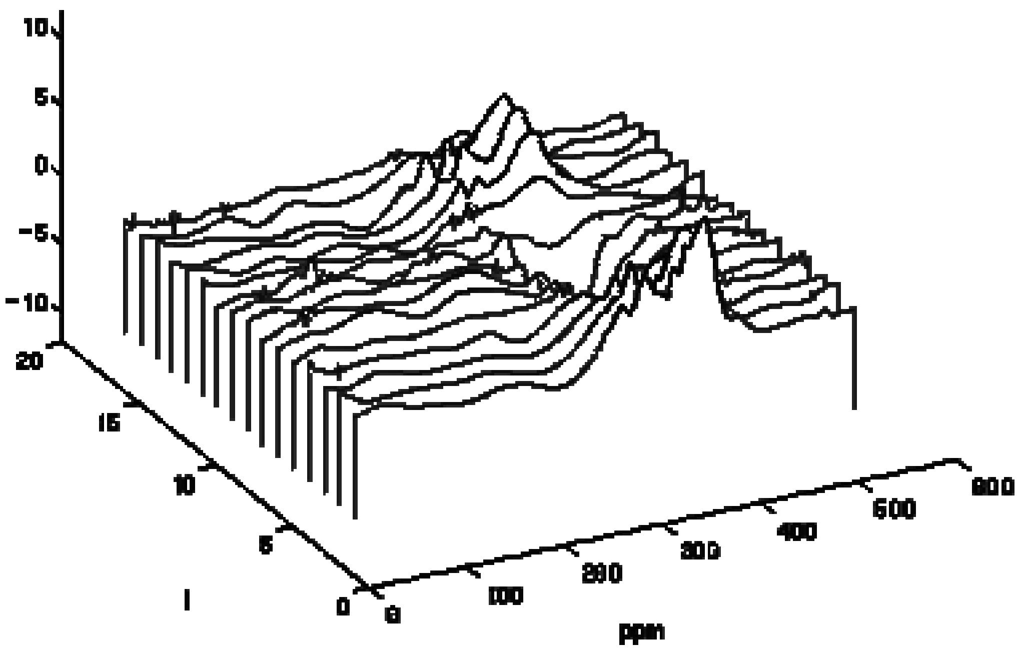

Figure 2. De-noised spectrum of Fig. 1 by wavelet shrinkage.