Regularized Spectral Lineshape Deconvolution

Y. Zhang[1], S. Li[1], and J. Shen[1]
[1]National Institute of Mental Health, Bethesda, Maryland, United States

Introduction Quantitative analysis of in vivo Magnetic Resonance Spectroscopy (MRS) is often hampered by lineshape distortions resulting from the magnetic field B_0 inhomogeneities and eddy currents. The knowledge of lineshape is therefore needed for spectral quantifications, especially in the presence of overlapping resonance lines. Although a model function can be used to fit a non-analytical lineshape and incorporated into the parametric analysis [1], this approach requires extra fitting parameters and has the tendency to result in unstable solutions. An preferred alternative is the deconvolution with methods such as the QUALITY (quantification improvement by converting lineshapes to the Lorentzian type) which use the water line shape as the reference to deconvolve the distortions and restore the Lorentzian type lineshape [2]. However, the time domain data division during the deconvolution causes the noise amplification for the portion of the data at the end of the time domain. Especially, the zero-division would occur at points where the reference signal has near zero values. Although a strongly decaying filter can be applied after the deconvolution to suppress the noise, it will broaden the line width. A cross-over point in the time domain was defined in a later developed method [3] in which only phase correction was performed after the cross-over point in order to prevent noise explosion. Here we proposed a new method which uses Tiknohov regularization [4] to restrain noise amplification.

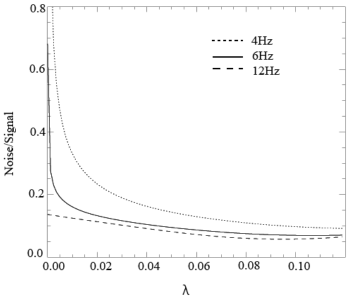

Fig. 1: L-curves of different line broadening factors. A λ value on the corner is used for the regularization parameter. A large λ is required to reduce the noise if line broadening filter is not strong enough to suppress the noise, while a small λ is preferred to preserve true Lorentzian lineshape.

Theory and Method We assume that *Y* is the observed signal with lineshape distortions and is to be deconvolved into *X* that decays exponentially, i.e.,

$$A(t_i)X(t_i) = Y(t_i) \qquad [1],$$

where $A(t_i)$ is the lineshape function described by the reference data, and t_i is time at the *i*th data point. Because the phase correction can be performed in a separate processing step, $A(t_i)$ here contains only the amplitude part of the reference data, and therefore $A(t_i) > 0$. The conventional solution to $X(t_i)$ is simply

$$X(t_i) = A^{-1}(t_i)Y(t_i) \qquad [2],$$

$A^{-1}(t_i)$ is the inverse of $A(t_i)$. Both $A(t_i)$ and $Y(t_i)$ contain the noise errors, which propagate to $X(t_i)$ by Eq.2. The noise errors will be significantly amplified at the points where $A(t_i)$ nears singular. Eq.2 may not be a desired solution as the resultant spectrum bears much more noises than the spectrum without deconvolution processing. The solution of Eq.2 is equivalent to minimizing the residual of the norm $\| AX - Y \|^2$. According to Tikhonov regularization, it should be replaced with

$$\min \| AX - Y \|^2 + \lambda \| X \|^2 \qquad [3],$$

which has the solution

$$X(t_i) = \frac{1}{A(t_i) + \lambda} Y(t_i) \qquad [4],$$

where λ is a positive regularization parameter to be determined later. Obviously, a non-zero λ eliminates the zero-division and restrains the noise amplification resulting from small values of $A(t_i)$. However, a minimal λ is preferred for complete lineshape restoration, because a large λ makes lineshape deviate from the Lorenzian type. We used the ratio of noise to signal in frequency domain versus the regularization parameter to plot the L-curve in determination of the optimal λ, as shown in Fig.1. There exists a transition point along the each curve where the noise level starts to increase abruptly. The amplitude of the reference data was normalized by its value at t_0, i.e., $A(t_0) = 1$. Because the noise level in frequency domain also depends on the line broadening applied in the time domain, the selection of the optimal λ requires an estimate of line broadening. The proposed method was validated on the data acquired on GE's 3T Excite scanners using the standard quadrature head coil and a PRESS sequence. The unsuppressed water reference scans were performed immediately after the spectral data collection.

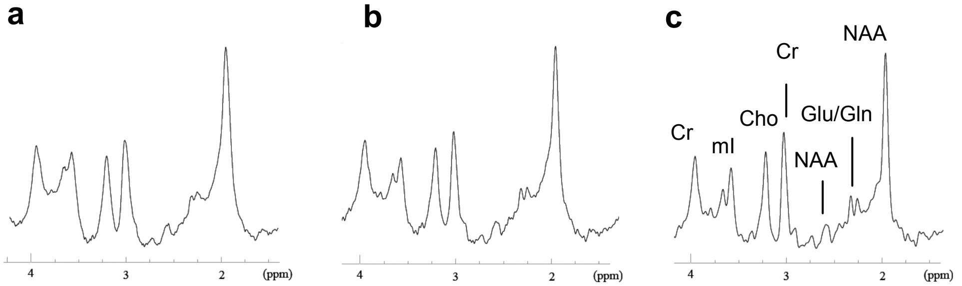

Fig.2: Comparison of different processing; a) without deconvolution; b) deconvolution without regularization; c) regularized deconvolution.

Results and Discussion The spectra in Fig. 2 were collected with the echo time of 35 ms from a frontal lobe voxel of human brain. Figure 2a is the original spectrum (line broadening = 1.5Hz) without lineshape correction. The improvements on resolution and lineshape are noticeable after the regularized deconvolution, as shown in Fig. 2c, which was obtained with a λ = 0.02 and line broadening factor = 6Hz. In Fig. 2b, without the regularization, i.e., λ = 0, a strong line broadening (10Hz) had to be applied in order to increase the signal to noise ratio to the level comparable with the other two spectra, and thus the benefit of lineshape deconvolution is considerably compromised. The λ of 0.02 is a point on the L-curve (solid line in Fig. 1) where the noise is about to increase dramatically. The process of lineshape deconvolution is an inverse problem. The use of regularization provides an optimal solution to the deconvolution; the noise is effectively reduced while the resultant lineshape is significantly improved with negligible bias.

References **1**. SW Provencher. Magn. Reson. Med. 1993;30:672-679. **2**. AA de Graff, *et al*. Magn. Reson. Med. 1990;13:343-357. **3**. R Bartha, *et al*. Magn. Reson. Med. 2000;44:641-645 **4**. AN Tikhonov. Soviet Math. Dokl. 1963;4:1624-1627.