A Note on the Accurate Model-based Spectral Fitting of Proton MRS in the Frequency Domain

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Introduction

In vivo MR signal is acquired as a discrete time series of the FID and can be analyzed either in the time domain (TD) or in the frequency domain (FD). However, the analytical equations of the MRS in the FD used for spectral fitting are obtained by continuous Fourier transform (CFT) of the corresponding functions in the TD. A simplified CFT expression for Loerentzian and Gaussian lineshapes, respectively, is as follows,

$$S_i(f) = a_i \frac{W_i^2}{W_i^2 + 4(f - f_i)^2}, \quad S_i(f) = a_i \exp(-\ln 2 \frac{4(f - f_i)^2}{W_i^2}) \qquad \text{(Eq. 1)}$$

where a_i, W_i and f_i are the height, FWHM and frequency of peak *i*, respectively. For both lineshapes, there is intrinsic difference between the CFT generated and DFT generated spectra (Fig. 1). The area under a peak in the CFT spectrum is ½ of that in the DFT spectrum. These differences may result in systematic errors when fitting the MR spectrum using these analytic equations. Although these errors can be eliminated by a simple procedure that removes the offset of the MR spectrum, they are often overlooked in practice, especially in fitting long TE MRS. In this work, we first employed computer simulations to show the errors if these differences are not addressed in the FD spectral fitting and the effectiveness of the procedure removing the offset. We further presented these comparisons using phantom and in vivo experiment data.

Methods

Computer simulation The synthesized FID consists of 4 spectral lines with their amplitudes to be 20, 40, 60 and 100, respectively, and their frequency relations close to the singlets of Cr, Cho, NAA and lipid at 3T. Two noise-free FID sets were synthesized with Lorentzian or Gaussian lineshape. Each FID was added with 500 sets of Gaussian noise with the same standard deviation, to form 500 datasets. We fitted the synthesized datasets in the TD and FD, respectively. For FD fitting, we fitted the spectrum with or without the offset, respectively. The offset was determined by averaging the data points from real (or imaginary) part of the spectrum in the peak-free region and subtract it from the DFT spectrum. After each fitting, the spectral lines were reconstructed separately, using the fitted parameters, and their peak areas were calculated.

Phantom and in vivo applications A phantom and a human measurement were performed on a 3T MR scanner (General Electric). MRSI data were acquired with the MPCSI pulse sequence [1]. Some parameters are FOV = 24x24 cm^2; PE = 16x16; and TR/TE = 2300/144 ms.

Data processing MRSI was reconstructed using 2D FFT with spatial filtering. Residual water signals were removed from the time domain data in the selected voxels by applying a high-pass filter. For FD spectral fitting, we zero-filled the TD signals to 2048 complex points and apply inverse FT to transform them to frequency domain. Model based parametric spectral fittings were performed using different models of Lorentzian, Gaussian and a simplified Voigtian [2], respectively. Spectral parameters were determined using a non-linear least squares algorithm. Fitted spectral data were reconstructed from the parameters and the models. All programs are written in Matlab.

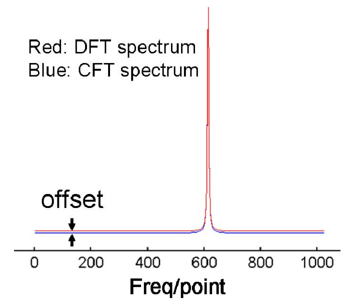

Fig.1. The offset between DFT and CFT spectra.

Tab.1. Means and SDs of the estimated peak areas using 3 different fitting procedures (for Lorentzian lineshape). Note the theoretical peak areas are 10, 20 and 30 for the FD model; and 20, 40 and 60 for the TD model.

Lines	1	2	3
TD	19.96+/-0.23	40.02+/-0.23	60.00+/-0.23
FD with offset	11.45+/-0.19	21.21+/-0.17	31.36+/-0.18
FD w.o offset	9.96+/-0.17	19.99+/-0.17	29.90+/-0.17

Results

Means and standard deviations of the estimated peak areas using different fitting procedures, i.e., TD fitting, FD fitting with offset and FD fitting without offset, are shown in the Table (only for Lorentzian lineshape as an example). The TD fitting gave results that are very close to the true values. The FD fitting with offset overestimates peak areas, which are ½ of their corresponding true values, by14.5%, 6.0% and 4.5%, for peak 1, 2, and 3, respectively. If one of the peaks, e.g., peak 1, is chosen as a reference, the errors of ratios of the other two peaks to the reference peak would be 17.0% and 15.5%, respectively. On the other hand, the FD fitting without offset significantly reduced the systematic errors. For example, the relative errors are 0.4%, 0.0% and 0.3% for the Lorentzian model. We also found that the fitting of the Gaussian lineshape is more robust and accurate than that of the Lorentzian lineshape in the presence of Gaussian noise [3]. A total of 130 voxels were selected from a slice in an in vivo MRSI and were fitted with the Voigtian model. The relative differences of estimated peak areas with offset with respect to those without offset are 17.8%, 13.5% and 4.4%, for Cho, Cr and NAA, respectively. An example of the spectral fitting is shown in Fig.2.

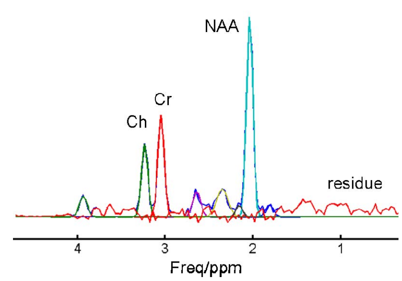

Fig.2. An example of the FD spectral fitting.

Discussion and conclusion

The offset between DFT spectrum and CFT spectrum will cause systematic errors in the DF spectral fitting. Although the baseline correction commonly used in the short TE spectral fitting can eliminate these errors, they are often overlooked in long TE MR spectral fitting, as the baseline is flat. These errors will persist and accumulate in the ratios of peak areas. The present result shows that the baseline correction or the offset removal is necessary, not only for the absolute peak area fitting but also for the calculation of the ratio of peak areas in long TE MRS.

References

[1] Duyn, J.H. et al. Radiology, 1993, 188:277-82. [2] Marshall, I et. al. MRM, 1997, 37:651-657. [3] Marshall , I et. al. MRM 2000, 44:646-649.