Lineshape Accommodation in Quantitation of Magnetic Resonance Spectroscopy Signals

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Introduction

Lineshape distortions due to residual eddy currents and magnetic field inhomogeneities are often present in short echo-time ^{1}H spectroscopic data. If left uncorrected, these lineshape distortions lead to errors in metabolite concentration estimates when using quantification methods that incorporate model functions with specific lineshapes (i.e., Lorentzian or Gaussian). Several methods have been proposed for lineshape correction, 1) The distorted *in vivo* signal can be given a purely Lorentzian lineshape by using methods such as QUALITY deconvolution and eddy current correction (ECC) or the hybrid method QUECC, see [1] and references therein. These methods use a separate reference spectrum for lineshape correction, for instance unsuppressed water; 2) The lineshape distortions with respect to the basis-set spectra are corrected in the fitting procedure, see *e.g.*[2, 3]. In this study a new method is investigated, namely the lineshape of the *simulated* metabolite basis-set signals is given the estimated lineshape of a reference spectrum before the quantitation step. Analytical formulae for the Cramér-Rao lower bounds (CRBs) on model function parameters of a Lorentzian and Gaussian singlet are also derived and provide insights in the lineshape accommodation strategy to be used.

Method

Monte Carlo Studies: The influence of different lineshape accommodation strategies on QUEST [2] quantitation results are investigated through Monte-Carlo studies. To assess the performances – including bias – of QUEST, a ^{1}H signal (2048 data points) mimicking an *in vivo* spectrum of rat brain at 9.4 Tesla was simulated, see Fig.1. This signal comprises contributions from eleven metabolites and lipids whose amplitudes correspond to a healthy rat-brain. Voigt lineshapes were imposed (damping factor of the form $\exp(-\alpha t - \beta t^2)$). The damping factors of the Lorentzian part range from 5Hz to 20Hz and that of the strong Gaussian part is 4 s^{-2}. To this simulated noiseless signal, 200 different realisations of white Gaussian noise were added. The noise level was chosen as in *in vivo* conditions so that the SNR of the Cr singlet be 8.6:16.

Quantitation: Signals were processed in the time domain. The metabolite basis-set signals used in QUEST were simulated with NMR-SCOPE using spin parameters given in [3]. Eleven metabolites – aspartate (Asp), choline (Cho), creatine (Cr), γ-amino-butyric acid (GABA), glucose (Glc), glutamate (Glu), glutamine (Gl), myo-Inositol (mI), N-acetylaspartate (NAA and NAAG), taurine (Tau) and lipids (Lip) at 0.9 and 1.3 ppm – were included. Three methods were investigated and compared, 1) a Lorentzian basis-set is used, 2) the Monte Carlo signals were given a purely Lorentzian lineshape using a deconvolution approach prior to quantitation and the basis-set was Lorentzian too, 3) an '**adapted**' basis set which was given the Voigt lineshape of a reference singlet, was used. Note that without reference, the lineshape signal can also be estimated from the data.

Analytical Formulae for the Cramér-Rao Bounds on Model Parameters of a Singlet

To help in finding the best lineshape accommodation strategy for quantitation, we derived (with Maple) analytical formulae for the CRBs on parameters of a singlet having a Lorentzian and a Gaussian lineshape respectively. The CRB on the amplitude of a Gaussian singlet is equal to $\sqrt[4]{18/\pi}\,\sigma\sqrt{ts}\sqrt[4]{\beta}$ where β is the damping factor of the Gaussian singlet, σ is the noise standard deviation and t_s the sampling interval. For a Lorentzian singlet, the CRB on the amplitude is $2\sigma\sqrt{ts}\sqrt{\alpha}$. The damping factors of Lorentzian and Gaussian singlets having the same amplitude and the same line width at half height, are such that $\beta = \alpha^2/4\ln 2$. The corresponding ratio of the CRBs on amplitudes is equal to $\mathrm{CRB}_{\mathrm{Lorentz}}/\mathrm{CRB}_{\mathrm{Gauss}} = (2/\sqrt{3})(2\pi\ln 2)^{1/4} \cong 1.668$. The quantitation error is then almost 40% lower for a singlet with a Gaussian lineshape. This result induced us to investigate whether it is advantageous to give the basis-set signals the estimated damping factors of a reference peak rather than to give the distorted *in vivo* signal an ideal Lorentzian lineshape by using a 'reference-deconvolution' algorithm.

Results

The 200 Voigt noisy signals were quantitated with QUEST using the three mentioned approaches. Figs. 2 shows the main Monte-Carlo results. The mean amplitudes of metabolites and one standard deviation estimated from the 200 signals are displayed. In semi-parametric estimation, bias is unavoidable. NAA and Cr have biased amplitude estimates when the Lorentzian basis-set is used. Using a deconvolution algorithm prior to the quantitation step does not remove the bias. The latter is reduced when using the adapted basis-set.

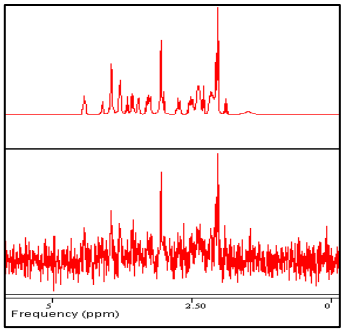

Fig. 1 QUEST quantitation results with jMRUI of a simulated spectrum mimicking a rat brain signal at 9.4 Tesla and used in the Monte Carlo study (top, estimated spectrum).

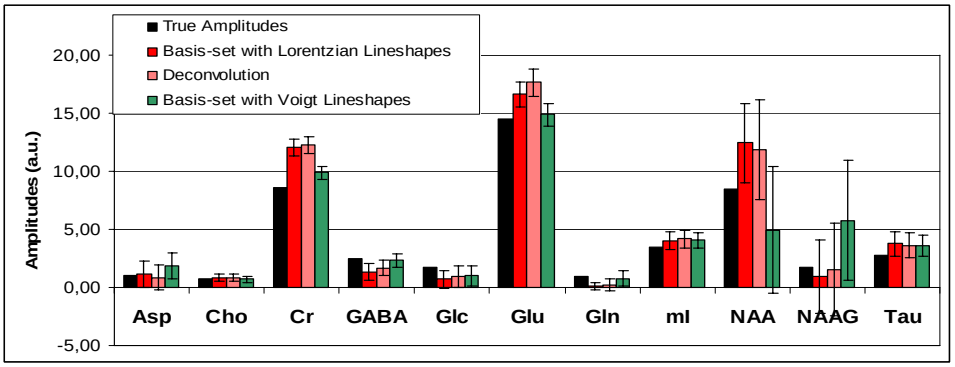

Fig. 2. Monte-Carlo studies. True amplitudes (black) and mean amplitudes of metabolites quantitated with QUEST for the three lineshape accommodation strategies. The error bars correspond to one standard deviation.

Conclusions

We studied the influence of lineshape distortions on quantitation results when using a fitting algorithm based on a metabolite basis-set. Giving the unknown lineshape of a reference peak to the metabolite basis-set lineshape seems preferable from our present Monte Carlo studies.

Acknowledgments: This work is supported by Philips Medical Systems, Best, NL, and the EU Marie Curie Research Network 'FAST', MRTNCT-2006-035801.

References

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