Spectral fitting in MRS: Uncertainties of parameter estimates for semi-parametric MR spectrum modelling

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Introduction

In processing of MR spectra Cramér-Rao lower bounds are often used to characterize the precision of parameter estimates attainable when applying parametric models to describe the spectra. However, for spectra acquired at shorter echo times, exhibiting non-negligible background features due to macromolecules and lipids, modern spectral processing includes some kind of (heuristic) background fitting, either parametrically or non-parametrically. In either case Cramér-Rao lower bounds may be of limited usefulness since the chosen background models may include model errors that are not accounted for. The necessity of accomodating the uncertainty of the background in an uncertainty measure of the estimates of the desired model parameters has recently been appreciated [1]. Using our semi-parametric MR spectrum processing method [2] we determined uncertainties of the parameter estimates by accounting for the additional uncertainty due to the background model.

Methods

The semi-parametric MR spectrum processing method [2] is a time domain-frequency domain procedure using a regularization method for non-parametric estimation of the background in the frequency domain. The uncertainties of the estimates of the parametric spectrum model are calculated as follows: First the covariance matrix of the estimates of the parameters (amplitudes, linewidths, phases) is determined for fixed regularization parameter. This step includes the increased uncertainty of the parameter estimates due to the simultaneous background modelling. In the second step a diagonal matrix is added to the covariance matrix which accounts for errors of the chosen regularization parameter and the background model. This diagonal matrix is determined by the variation of the resulting parameter estimates for reasonable changes of the regularization parameter. The method has been checked by applying it to simulated spectra of varying background and different SNRs. Calculated uncertainties were found to reflect resulting root mean square errors of parameter estimates well.

In vivo proton MR spectra were measured in 11 healthy volunteer brains on a Medspec 30/100 scanner (Bruker Biospin, Ettlingen, Germany) at a field strength of 3 T using a circularly polarized head coil. Volumes of interest measured 20 x 30 x 20 mm^3 and contained the left hippocampus. After manual shimming on the voxel to a water resonance linewidth of 6 - 7 Hz, and 90°-pulse calibration, PRESS spectra were acquired using Shinnar-LeRoux-optimized 90° and Mao 180° pulses with T_R = 3 s and T_E = 80 ms. Metabolite concentrations were determined from amplitudes as described in Ref. 2.

Results and Discussion

The simulations showed that the necessity of considering the uncertainty of the background treatment grows as both the size of the background and the SNR grow. In order to study this influence for real data Fig. 1 depicts mean uncertainties obtained for fitting total creatine, total choline, NAA, glutamate and glutamine to 11 in vivo spectra; both total uncertainties of the obtained concentrations and those solely due to the uncertainty of the background model are shown. A considerable fraction of the uncertainty due to the background model is observed for the singlets, which intrinsically exhibit large SNR.

Inclusion of background model uncertainty adds useful information to uncertainty measures and appears important for evaluating goodness of fit and comparing different fitting methods. The (relative) influence of the background model uncertainty increases with increasing SNR, which may be expected since in case of vanishing statistical errors only the model error of the background remains as the source of uncertainty. Moreover, our study shows that even at the echo time of 80 ms, where background features appear less pronounced to visual inspection, the contribution of the uncertainty of the background model cannot be neglected.

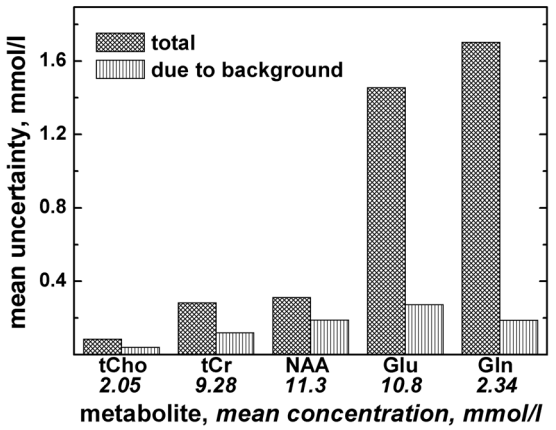

Figure 1: Mean uncertainties for estimation of 5 metabolites in a human hippocampus voxel (n = 11).

References

1. Ratiney H et al, Proc 20th ESMRMB Meeting, Rotterdam 2003, 272.
2. Schubert F et al, NeuroImage, in press.