Two-Dimensional J-resolved Spectroscopy Fitting

R. F. Schulte1, P. Boesiger1

1Institute for Biomedical Engineering, University and ETH Zurich, CH-8092 Zurich, Switzerland

Introduction

J-coupled metabolites are generally difficult to detect and quantify in vivo. Promising approaches are spectral editing and multi-dimensional spectroscopy. A simple and useful 2D sequence providing better distinction of the J-coupled resonances is 2D J-resolved spectroscopy (JPRESS) [1]. The maximum information contained in the spectra can be extracted through fitting directly in two dimensions with all the prior knowledge available. A first attempt to fit in 2D was made through the 2D Hankel singular value decomposition [2], which fails to yield satisfactory results for in vivo JPRESS spectra due to experimental imperfections, the impossibility to impose prior knowledge and other conceptual shortcomings. Another attempt was made through fitting 2D spectra as constrained 1D fits [3] without Fourier transforming the indirect dimension. However, this was only applied to glutamate phantoms yielding limited benefits. In this work a fully two-dimensional fitting procedure is presented, which is capable of applying the complete prior knowledge available. In vivo T2 relaxation times are directly obtained for a wide range of metabolites.

Theory and Methods

The 2D fitting procedure is based on two complementary approaches - LCModel [4] for providing the maximum prior knowledge constraint and VARPRO [5] for minimising the degrees of freedom. The JPRESS spectra are fitted in the frequency domain, mainly because of convenience of implementation. A linear combination of model spectra approximates the measured spectrum based on the following optimisation parameters: individual for each metabolite are the concentration, line broadening and a small chemical shift. The global parameters for the whole spectrum are the phase and a line shape distortion function. Several strategies are applied to restrict the numerous degrees of freedom. The fitting is split up (Fig.1) - similar to VARPRO [5] - into a non-linear outer loop for optimising the non-linear parameters, such as line broadening and phase. In an inner step, the basis spectra are updated to the given parameters from the outer loop. The spectrum is approximated by this basis through a linear least squares fit, yielding the individual concentrations. Since the concentrations are not optimised in the outer loop, the degrees of freedom are reduced and the robustness is increased compared to a complete non-linear fit. Further strategies for a successful fit are a good initialisation, starting close to the minimum and repeating the fitting procedure four times, each time with increasing the degrees of freedom and initialisation with the result of the preceding step. The basis spectra were simulated numerically with the GAMMA library [6]. All experiments were performed on a Philips Intra 3T scanner equipped with a transmit/receive head coil. Twenty-seven healthy volunteers with written informed consent (age 35.4±7.5) were measured in the parietal lobe. PRESS was acquired with $T_E=31$ ms, $T_R=2.5$ s and 256 averages for comparison with LCModel [4]. JPRESS was acquired with $T_E=31$ to 229 ms, $T_R=2.5$ s, 100/2048 samples in $t_1/t_2$, BW=0.5/2 kHz in $f_1/f_2$ and a four-step phase-cycling scheme. The data was eddy current corrected, reconstructed to $J$-resolved Spectroscopy Fitting

Discussion and Conclusion

The direct 2D fitting of JPRESS is a useful and promising approach for the in vivo detection and quantification of many J-coupled metabolites, which are currently difficult if not impossible to assess. The underlying limitation in 2D is not governed by the overlap of metabolites any more, but rather by sensitivity. The whole procedure is fully automatic and easily applicable even in the clinical routine. A big advantage over other forms of editing is the estimation of the individual quantification errors through the Cramer-Rao lower bound.

The baseline in JPRESS is flat and well-behaved and was not included in the fit, hence reducing the uncertainty of the fit. This might explain the differences in concentrations to LCModel [5], where the baseline is modelled through broad singlets and splines. Furthermore, different relaxation behaviour inside the measured basis spectra might underestimate the concentrations of metabolites with short T2 times in case of LCModel, as the PRESS echo time is about half the in vivo T2 relaxation. As one usually looks at concentration changes in spectroscopy, this consistent difference is unproblematic.

References
