Semi-Parametric Estimation in Magnetic Resonance Spectroscopy: Automation of the Disentanglement Procedure

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Introduction

Magnetic Resonance Spectroscopy (MRS) is a unique tool for non-invasive *in vivo* detection and quantitation of metabolites. A point of concern is disentanglement of perturbing – macromolecules and lipid - signals from the wanted metabolite signals. We derived Cramér-Rao bounds (CRBs) on the data-points of the perturbing signals. Exploiting the attendant formulae, we show that it is possible to automate – for use in clinics – the disentanglement procedure in the metabolite quantitation algorithm 'QUEST' ([1]), part of the freely available MRS software jMRUI; `see http://www.mrui.uab.es/mrui/.`

Method

Disentanglement Procedure

An *in vivo* MRS signal, contaminated by a nondescript background signal due mainly to macromolecules and lipids, can be modelled by

$$x = \hat{x}_{\mathrm{Met}} + b + e\,, \qquad (1)$$

where $\hat{x}_{\mathrm{Met}}$ is the metabolite part whose model function is known, b the background signal whose model function is often only partially known, and e Gaussian-distributed noise. First, we truncate (omit) an appropriate number of initial data points. The resulting signal x_{trunc} can be modelled by $x_{\mathrm{trunc}} \approx \hat{x}_{\mathrm{Met}_{\mathrm{trunc}}} + e_{\mathrm{trunc}}$

After quantitation with QUEST, the residue approximates the noise because the background resides mainly in the omitted initial data points. Then, back-extrapolating $\hat{x}_{\mathrm{Met}_{\mathrm{trunc}}}$ to $t = 0$, one obtains an approximation of $\hat{x}_{\mathrm{Met}}$. Subtraction of the latter from the raw data, in turn yields a good approximation $\tilde{b}$ of the background signal plus noise, i.e., $\tilde{b} \approx x - \hat{x}_{\mathrm{Met}} = b + e\,.$ (2)

The number of data-points N_{trunc} used in the characterization of the background signal plays an important role in the quantitation procedure itself and needs to be automated.

Error estimation on the background data-points

Using Eq. 2 and the generalized CRB theorem pertaining to functions [2], we derived CRBs on the background complex valued data-points b_n, $n = 0, 1, \ldots, N_{\mathrm{trunc}}$. These CRB_{bn} and errors σ_{bn} can be written as

$$\sigma_{b_n} \geq \mathrm{CRB}_{b_n} = \sigma_{\mathrm{Noise}} \sqrt{(\mathbf{J}_1(\mathbf{J}_2^{\mathrm{T}}\mathbf{J}_2)^{-1}\mathbf{J}_1^{\mathrm{T}})_{nn}}\,, \qquad (3)$$

where the sizes of the Jacobian matrices $\mathbf{J_1}$ and $\mathbf{J_2}$ are $2N_{\mathrm{trunc}} \times P$ and $2(N - N_{\mathrm{trunc}}) \times P$ respectively. σ_{Noise} is the noise standard deviation estimated from the last data-points of the time domain signals. P stands for the number of parameters used in the parametric quantitation procedure.

Automation of the Disentanglement Procedure

Exploiting Eq. 3, we devised a procedure to automatically estimate the optimum value of N_{trunc}. Our criterion consists of finding the smallest value of n for which the following conditions are satisfied: $|b_n| < 1.4\mathrm{CRB}_{|bn|}$ and $|b_n| < \sigma_{\mathrm{Noise}}$.

Results

Monte-Carlo studies

The simulated signal (Fig. 1) comprised contributions from three metabolites, background and Gaussian noise, 256 different realizations of white Gaussian noise were consecutively added.

Automatic choice of the optimum number of truncated points

In Fig. 2, it can be seen that the background signal decays into the noise after the 23rd data-point. On the histogram of the occurrences of the optimum number of truncated data-points found from the 256 Monte-Carlo signals, the optimum value is 15 for 160 of them (see Fig. 3). Thus, there is a *trade-off* between a good fit of the background and a good fit of the metabolite signal.

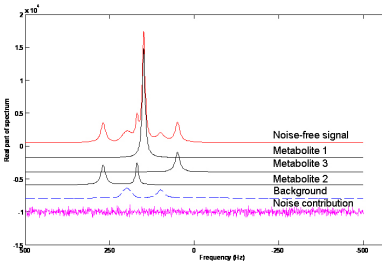

Figure 1: Fourier Transform of the noise-free MRS signal, the metabolite contributions, the background signal and noise.

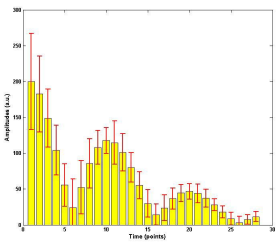

Figure 2: Error estimation on the background data-points obtained from the Monte Carlo study. Absolute value of the true background (yellow) and mean values of the corresponding estimated $\mathrm{CRB}_{|bn|}$ (28 truncated data-points were used).

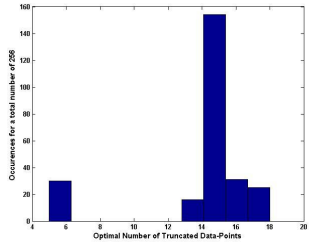

Figure 3: Histogram of the occurrences of the optimum number of truncated data-points found from the 256 noisy signals of the Monte Carlo study.

Conclusions

We investigated automation of the disentanglement procedure in QUEST. We distinguish two main goals

- Derivation of Cramér-Rao bounds on the errors of the estimated background data-points.
- Automatic choice of the optimal number of initial data-points to be used for modelling the background signal.

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References

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