Error Bounds For Semi-Parametric Estimation in MRS

H. Ratiney[1], E. Capobianco[2], R. de Beer[3], D. van Ormondt[3], D. Graveron-Demilly[1]

[1]Laboratoire de RMN, CNRS UMR 5012, Université Claude Bernard, Lyon I - CPE, Villeurbanne, France, [2]Biomedical Engineering, University of Boston, Boston, MA, United States, [3]Applied Physics, Delft University of Technology, Delft, Netherlands

Introduction

The theory of Cramér-Rao lower Bounds (CRBs) on errors in parameter estimates is valid only if the model function used for describing the data is physically correct. Thus, if the data contain a nondescript part indicated as `background' -- as with e.g. $^1$H short echo-time signals -- the usual CRBs become invalid [1,2,3]. In such cases, one has to resort to *semi*-parametric estimation, approximating the `non-parametric' background with some mathematical function (*i.e.* not derived from the physical phenomenon at hand). The estimation errors in the wanted parameters -- statistical and systematic -- depend on how one handles the non-parametric background. By varying the number of degrees of freedom allotted to estimating the background, one can trade-off variance with bias and thus seek a minimum of the root mean square errors of the wanted parameters. We propose error bounds that are independent of the way of estimating the background. To this end, we derive a new general result concerning CRBs. The proposed bounds are not absolute lower bounds, but rather upper bounds that should hold for a number estimators. The actual semi-parametric estimation errors are between the `usual' CRBs mentioned above and these upper bounds.

Method

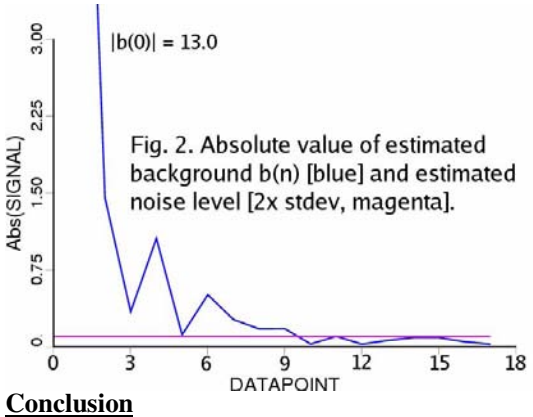
A broad nondescript background can be accommodated by adding unknown, complex-valued numbers b(n) to data-points $n = 0,1, \ldots, n_{bg}$ of the initial part of the time-domain model function [4]. The subscript $_{bg}$ stands for background. For $n > n_{bg}$, these numbers are small enough wrt the noise level to be neglected. The n_{bg} numbers *b(n)* can be treated as $2n_{bg}$ *free*, real-valued parameters and included in the estimation procedure (model fit) in natural fashion. An important step in parameter estimation and CRBs is to set up the Jacobian matrix **J.** We partitioned **J** as shown in Fig. 1. $\mathbf{J}_1$ and $\mathbf{J}_2$ pertain to the metabolite parameters, for $n \leq n_{bg}$ and $n > n_{bg}$ respectively; the unit matrix $\mathbf{I}_{bg}$ pertains to the background parameters/signal *b(n)*; **0** is a zero matrix. The form of the partitioned Fisher matrix **F** is straightforward. In order to minimize influence of estimation methods, no regularization of the values of *b(n)* is imposed.

Results

The CRBs are the diagonal elements of the matrix $\mathbf{F}^{-1}$. Fig. 1 shows the general analytic solution of this inverse. To the best of our knowledge this result is new. The CRBs of the metabolites are in the upper left partition, made up of $(\mathbf{J}_2^T\mathbf{J}_2)^{-1}$. The latter is exactly what one would get for $\mathbf{J} = \mathbf{J}_2$ which pertains to retaining only the data-points $n > n_{bg}$ where the background has decayed to below the noise level and can be neglected, *i.e.*, simple truncation of the part where background and metabolites are entangled.

$$\mathbf{J} = \begin{array}{|c|c|}\hline \mathbf{J}_1 & \mathbf{I}_{bg} \\ \hline \mathbf{J}_2 & \mathbf{0} \\ \hline \end{array}, \quad \mathbf{F} = \mathbf{J}^T\mathbf{J} = \begin{array}{|c|c|}\hline \mathbf{J}_1^T\mathbf{J}_1 + \mathbf{J}_2^T\mathbf{J}_2 & \mathbf{J}_1^T \\ \hline \mathbf{J}_1 & \mathbf{I}_{bg} \\ \hline \end{array}, \quad \mathbf{F}^{-1} = (\mathbf{J}^T\mathbf{J})^{-1} = \begin{array}{|c|c|}\hline (\mathbf{J}_2^T\mathbf{J}_2)^{-1} & -(\mathbf{J}_2^T\mathbf{J}_2)^{-1}\mathbf{J}_1^T \\ \hline -\mathbf{J}_1(\mathbf{J}_2^T\mathbf{J}_2)^{-1} & \mathbf{I}_{bg} + \mathbf{J}_1(\mathbf{J}_2^T\mathbf{J}_2)^{-1}\mathbf{J}_1^T \\ \hline \end{array}.$$

Fig.1. Partitioned matrices **J** (Jacobian), **F** (Fisher), and $\mathbf{F}^{-1}$ (CRB). $\mathbf{J}_1$, $\mathbf{J}_2$ are for $n \leq n_{bg}$, $n < n_{bg}$. $\mathbf{I}_{bg}$ is a unit matrix.



Computation of the metabolite CRBs from the disentangled part of the signal, i.e. for $n > n_{bg}$, is quick and easy. Fig. 2 shows the estimated background *b(n)* and estimated noise level of a simulated signal MRS signal, enabling in turn to estimate n_{bg}. Our simulations indicate that the CRBs of heavily overlapping multicomponent metabolites on a background, calculated from $(\mathbf{J}^T_2\ \mathbf{J}_2)^{-1}$, can be up to 5 times higher than CRBs calculated without influence of a background and using all data-points. The only knowledge used was that a broad background decays quickly into the noise at some early sample number n_{bg}, the estimation of which is not too complicated. The extended CRBs derived here can be considered as upper bounds because all metabolite information contained in data-points $n \leq n_{bg}$ has been ignored.

Conclusion

We derived a simple, *general* expression for CRBs that includes full (not regularized) parametrization of the background and can be used as upper bounds of semi-parametric} metabolite estimation errors. It enables evaluation of improvements achieved with regularization imposed on *b(n)*.

Acknowledgment This work is supported by Philips Medical Systems, Best, NL.

References

[1] H. Ratiney *et al*, Proc. Intl. Soc. Mag. Reson. Med., **12**:306 (2004). [2] J.C. Spall, Proc. Amer. Control Conf. **4**:3140-3145 (2004). [3] C. Elster *et al*, Magn. Reson. Med., **53**:1288-1296 (2005). [4] E. Weiland *et al*, Proc. Intl. Soc. Mag. Reson. Med., **11**:1160 (2003).