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SVD-BASED MODELLING OF MEDICAL NMR SIGNALS

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ABSTRACT. A Magnetic Resonance (MR) scanner enables one to noninvasively detect and quantify biochemical substances at selected positions in patients. The MR signal detected by the scanner comprises a number of damped sinusoids in the time domain. Each chemical substance contributes at least one sinusoid, at a specific frequency. Often, metabolite quantification is severely hampered by interference with strong MR signals of water and other substances (*e.g.* fat) resident in the human body. The damping function of the interfering sinusoids is nonexponential, which aggravates the situation. We investigate subtraction of interfering sinusoids by means of SVD-based state space modelling. Among other things, modelling of all details of the signal is attempted (zero-error modelling). Rank criteria for three alternative Hankel data matrices guaranteeing zero-error modelling, are provided. Measures to meet the criteria are proposed and tested on simulated signals. Although zero-error modelling can indeed be achieved, it turns out that such modelling does not guarantee exact separation of the unwanted sinusoids from the wanted sinusoids.

KEYWORDS. SVD, magnetic resonance spectroscopy, *in vivo*, state space, zero-error modelling

1 INTRODUCTION

A Magnetic Resonance (MR) scanner enables one to noninvasively detect and quantify biochemical substances at selected positions in patients [1]. Often the signal processing attendant on quantification is hampered by interference from MR signals of water and other substances (*e.g.* fat) resident in the human body. Removal of such signals prior to the quantification step is desired. Fig. 1 shows a typical example, transformed from the measurement domain (= time domain) to the frequency domain by FFT for display reasons. See caption of Fig.1 for details.

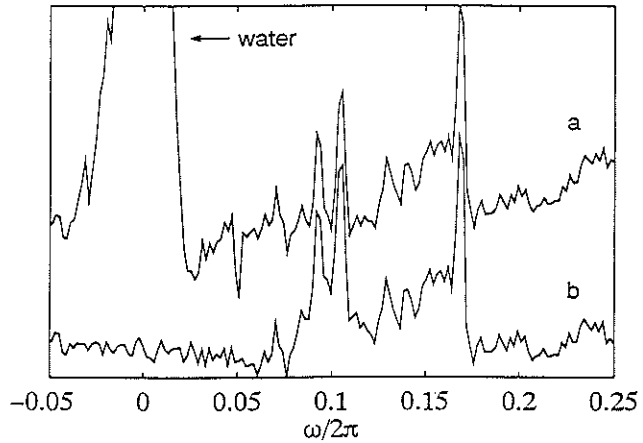


Figure 1: State space processing of an *in vivo* MR time domain signal from the right parietal lobe of a human brain. The results are displayed in the frequency domain by applying FFT and plotting the real part. a) The spectral region of interest of the raw data minus the two first data points which are corrupted. A huge unwanted peak of nondescript (*i.e.*, no model function available) shape originating from water dominates. b) Spectrum after subtraction of the water contribution as parametrized with seven sinusoids using the SVD-based state space algorithm of Kung *et al.* [2]. In addition, two relatively strongly damped sinusoids were subtracted at $\omega/2\pi$= 0.101 and 0.252, $\omega_{\text{Nyquist}} = \pi$. (Note that the mentioned omission of initial datapoints causes perturbation of the baseline that may be hard to distinguish from genuine MR features. This is a mere display problem.)

Apparently, Kung et al.'s SVD-based state space method [2] is capable of modelling nondescript (*i.e.*, model function unknown) components in terms of exponentially damped sinusoids. Other examples of this feat were shown in the recent past [3]. However, several important aspects of modelling nondescript signals are yet to be resolved. First, criteria guaranteeing success of the modelling seem lacking. This is crucial in the context of automated processing of large numbers of signals. Success is defined here as the degree to which all details of the data can be accounted for. Ref.[4] advocates 'zero-error modelling', which aims to reduce the residue of model minus data to zero. Second, little is known about the extent to which successful modelling yields the true physical parameters. This is important for establishing whether removal of unwanted components from the signal by subtracting the related part of the model does affect the wanted components. In the present contribution we address both aspects.

2 METHOD

2.1 PRELIMINARIES

For reasons of space, we assume that the reader is familiar with the essence of Kung et al.'s SVD-based state space method [2, 5, 6, 7]. We recall that the starting point of the method is rearrangement of the complex-valued data x_n, $n = 0, 1, \ldots, N-1$, into an $L \times M$ Hankel data matrix X whose elements are $X_{l,m} = x_{l+m-2}$, $l = 1, 2, \ldots, L$, and $m = 1, 2, \ldots, M$, and $L + M = N + 1$, *i.e.*

$$X = \begin{pmatrix} x_0 & x_1 & x_2 & \cdots & x_{M-1} \\ x_1 & x_2 & & \cdots & x_M \\ x_2 & & & & \\ \vdots & \vdots & & & \vdots \\ x_{L-1} & x_L & & \cdots & x_{N-1} \end{pmatrix}. \tag{1}$$

Next, X is subjected to SVD, according to $X = U\Lambda V^H$. If the signal x_n comprises K exponentially damped sinusoids, $c_k \exp[(\alpha_k + i\omega_k)n]$, and no noise, the rank of X equals K ($k = 1, 2, \ldots, K$, with $K \leq L, M$; $i = \sqrt{-1}$). The frequencies ω_k and damping factors α_k can easily be estimated from the K leading singular vectors of U or V [2], using linear least squares or total least squares [8]. The complex-valued amplitudes c_k can subsequently be estimated by linear least squares fitting of the sinusoids to the signal. Once the ω_k, α_k, and c_k have been estimated, a 'Vandermonde decomposition' of X has been accomplished [2], according to

$$X = \begin{pmatrix} z_1^0 & z_2^0 & \cdots & z_K^0 \\ z_1^1 & z_2^1 & \cdots & z_K^1 \\ & & & \\ \vdots & \vdots & & \vdots \\ z_1^{L-1} & z_2^{L-1} & \cdots & z_K^{L-1} \end{pmatrix} \begin{pmatrix} c_0 & & & \\ & c_1 & & 0 \\ & & \ddots & \\ & 0 & & c_K \end{pmatrix} \begin{pmatrix} z_1^0 & z_1^1 & \cdots & z_1^{M-1} \\ z_2^0 & z_2^1 & \cdots & z_2^{M-1} \\ \vdots & \vdots & & \vdots \\ z_K^0 & z_K^1 & \cdots & z_K^{M-1} \end{pmatrix}, \tag{2}$$

with $z_k \stackrel{def}{=} \exp(\alpha_k + i\omega_k)$, $k = 1, 2, \ldots, K$. For later use, we mention that the model function for each data point can be expressed as

$$x_n = \sum_{k=1}^{K} c_k z_k^n \tag{3}$$

For the purpose of making a robust automated estimator based on the above, it is important to know whether the rank statement is reversible, i.e. does $\mathrm{Rank}(X) = K$ always imply that the signal comprises K sinusoids? The answer is negative. In view of this we propose a simple 'regularization' of the SVD-based state space method that should render all conceivable signals tractable, albeit at a cost.

2.2 RANK CRITERION FOR SUCCESSFUL MODELLING

In this subsection we indicate without our proof how one can establish whether state space modelling is capable of zero-error modelling the given data. To this end we write two additional data matrices that differ from the one defined in Eq.(1), through their numbers of rows and columns. (If L and M are specified, either X' or X'' can be dropped.)

$$X' = \begin{pmatrix} x_0 & x_1 & x_2 & \cdots & x_{M-1} \\ x_1 & x_2 & & \cdots & x_M \\ x_2 & & & & \\ \vdots & \vdots & & & \vdots \\ x_{L-2} & x_{L-1} & & \cdots & x_{N-2} \end{pmatrix}, X'' = \begin{pmatrix} x_0 & x_1 & x_2 & \cdots & x_M \\ x_1 & x_2 & & \cdots & x_{M+1} \\ x_2 & & & & \\ \vdots & \vdots & & & \vdots \\ x_{L-2} & x_{L-1} & & \cdots & x_{N-1} \end{pmatrix}. \quad (4)$$

Criterion for possibility of exact (i.e., zero-error) modelling:
If $\mathrm{Rank}(X) = \mathrm{Rank}(X') = \mathrm{Rank}(X'') = J$, with $J \leq \min(L-1, M)$, then it is possible to model data point x_n exactly as

$$x_n = \sum_{k=1}^{K} (\vec{c}_k)^T (\phi_k^n)^T \vec{u}_k \,, \quad (5)$$

where $J \stackrel{def}{=} \sum_k \mu_k \geq K$, ^{T} denotes transposition, $\vec{c}_k$ is a $\mu_k \times 1$ amplitude vector, ϕ_k is a $\mu_k \times \mu_k$ Jordan matrix, and $\vec{u}_k$ a $\mu_k \times 1$ unit vector:

$$\vec{c}_k = \begin{pmatrix} c_k^{(1)} \\ c_k^{(2)} \\ \vdots \\ c_k^{(\mu_k)} \end{pmatrix}, \quad \phi_k = \begin{pmatrix} z_k & 1 & & & \\ & z_k & 1 & 0 & \\ & & \ddots & \ddots & \\ & 0 & & z_k & 1 \\ & & & & z_k \end{pmatrix}, \quad \vec{u}_k = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \quad (6)$$

It can be seen that Eq.(6) reduces to Eq.(3) when all μ_k equal 1. If a signal comprises a time polynomial of order P, then $\mu_k = P + 1$. During execution of the algorithm, this becomes apparent through $(P+1)$-fold degeneracy of an eigenvalue of a Jordan matrix. However, a small amount of added noise already lifts the degeneracy. One must then consider whether to still model with a polynomial, or with P exponentially damped sinusoids. The latter aspect needs further research. For MR signals the given criterion can be strictly satisfied only by choosing $L - 1 = M = N/2$, assuming N is even. This is because in the real-world MR signals are corrupted by noise, and moreover, their damping is only approximately exponential. As a result, an MR data matrix most often has full rank, regardless of its size. The mentioned size choice yields $\mathrm{Rank}(X) = \mathrm{Rank}(X') = \mathrm{Rank}(X'') = N/2$. See also [9], page 167, and [4]. The modelling being full, it may enable one to remove unwanted features from the signal, which is the ultimate goal of this research.

2.3 REGULARIZATION

Removal of unwanted features is particularly useful if it can be fully automated, obviating the need of human intervention in *e.g.* a hospital environment. This requires numerical stability of the computations. Under the circumstances, it may be hazardous to trust that the noise present in the signal always guarantees full rank. Therefore we propose to provide the guarantee by adding a deterministic perturbation to the signal. The perturbation should be simple, so as to allow (future) analytical calculation of its effect. In this work the perturbation is $\epsilon(0, 0, \ldots, 0, 1, 0, 0, \ldots, 0, 1)$, where ϵ is an adjustable constant. This amounts to adding an outlier ϵ to data points no. $N/2 - 1$ and $N - 1$, N being even and the numbering starting at zero. In the sequel, this measure is called regularization. The resulting regularized data matrix, X_r, is

$$X_r = X + \epsilon \begin{pmatrix} & & & & 1 \\ & 0 & & 1 & \\ & & \cdot & & \\ & 1 & & \cdot & \\ 1 & & 0 & & \\ & & & & 1 \end{pmatrix}. \quad (7)$$

The ratio of the largest and smallest singular values of X_r can be set by varying ϵ. In this study the regularizing signal is simultaneously assigned the role of possible background signal which is to be subtracted after modelling has been achieved. Its N Fourier coefficients are alternatingly nonzero and zero, which results in considerable overlap with the spectrum of the wanted signal. Controlled overlap is desired in order to better study its effect on the state space estimates.

If all Jordan blocks have size $\mu_k = 1$, the original state space algorithm of Kung *et al.* can be applied. If $\mu_k > 1$, for one or more values of k, the model function must be adapted according to Eq.(6). The latter is required only in the second stage where the amplitudes are estimated. Once zero-error modelling has been achieved, the next task is to identify those sinusoids that represent the original wanted signal, and to evaluate the extent to which the unwanted components affect the estimates of the wanted parameters.

3 RESULTS AND DISCUSSION

The method described above was tried on a noiseless simulated signal comprising a single exponentially damped sinusoid perturbed by the 2 outliers ϵ, shown in Fig.2. Two cases, differing in frequency of the sinusoid, were considered. Details about the chosen parameters

and the results of the zero-error modelling are listed in Table1. For $\omega/2\pi = 0.1230$, the singular values of the 17×16 regularized data matrix X_r are $\lambda_1 = 7.644$, $\lambda_2 = 1.366$, λ_3 through $\lambda_{15} = 1.000$, $\lambda_{16} = 0.876$, which indicates that the rank of X_r is well defined and indeed full. Nearly the same singular values are found for $\omega/2\pi = 0.15625$. The small residues quoted

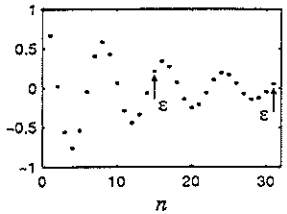


Figure 2: Simulated signal, comprising one noiseless, exponentially damped, sinusoid and two outliers of magnitude ϵ, at $n = 15$ and 31, indicated by arrows. Table 1 lists the results of zero-error modelling for $\epsilon = 1$ and two different frequencies of the sinusoid.

in the footnote of Table 1 show that zero-error modelling can be achieved. For both cases, the original sinusoid can be located at $k = 6$. Since all parameters have been estimated, subtraction of unwanted components on the basis of zero-error modelling is feasible. At the same time, this particular example shows limitations of the procedure. The estimates for $k = 6$ can be seen to deviate somewhat from the true parameters, listed immediately underneath. The deviations depend on the frequency, which is related to the fact that the power spectrum of the regularizing signal peaks at $\omega/2\pi = m/16$, $m = -8, -7, \ldots, 7$. For $m = 2$, $\omega/2\pi = 0.12500$, which is near 0.1230; for $m = 2.5$, $\omega/2\pi = 0.15625$. Apparently, the parameters are better when the frequency of the wanted sinusoid is close to that of an unwanted sinusoid. Note the 'reverse damping' and small initial amplitude for $k = 5$, $\omega/2\pi = 0.15625$. At present we can not yet offer quantitative explanations of the observed phenomena. An analytic state space solution for the simple signal of Fig.2 is sought. Finally, we point out that in real-world cases, it may be difficult to distinguish between a wanted component and an unwanted component occupying the same frequency region. It is unfortunate that prior knowledge about the wanted part of the signal, such as relative frequencies and phases, cannot yet be exploited by SVD-based state space modelling.

4 SUMMARY AND CONCLUSIONS

- Zero-error state space modelling is possible if the data matrix satisfies certain rank criteria. (Proof omitted for reasons of space.)
- A procedure for imposing the rank criteria (regularization) on the data matrix of an arbitrary signal, is devised. This regularization does not entail addition of random noise to the data.
- Our state space solution is not restricted to exponentially damped sinusoids.

- Zero-error state space modelling is capable of quantification of nondescript unwanted components in MR time domain signals. The spectrum of the unwanted components strongly overlaps with that of wanted components. The perturbation of parameter estimates of the wanted components is studied.

Table 1: Results of zero-error[a] SVD-based state space modelling for a single exponentially damped sinusoid augmented by two unit outliers as indicated in Fig.1. The true values of the sinusoid are listed below line $k = 6$. $L = 17$, $M = 16$, $N = 32$. $c_k = |c_k|\exp(i\varphi_k)$. Two frequencies are considered: $\omega/2\pi = 0.1230, 0.15625$, with $\omega_{\text{Nyquist}} = \pi$. $\epsilon = 1$.

k	$\lvert c_k\rvert$	$\varphi_k^{(0)}$	α_k	$\omega_k/2\pi$	$\lvert c_k\rvert$	$\varphi_k^{(0)}$	α_k	$\omega_k/2\pi$
1	0.0608	155.6	0.0017	0.4378	0.0723	166.2	-0.0092	0.4359
2	0.0611	132.4	0.0014	0.3755	0.0720	147.4	-0.0086	0.3727
3	0.0615	109.0	0.0008	0.3131	0.0719	131.0	-0.0077	0.3091
4	0.0624	84.8	-0.0003	0.2509	0.0732	122.6	-0.0059	0.2440
5	0.0653	58.1	-0.0039	0.1890	0.0039	-29.5	0.1464	0.1637
6	1.0270	0.6	-0.0617	0.1243	1.1638	13.0	-0.0937	0.1502
true	1.0000	0.0	-0.0670	0.1230	1.0000	0.0	-0.0670	0.15625
7	0.0596	32.9	0.0014	0.0607	0.0850	-5.1	-0.0163	0.0677
8	0.0594	4.6	0.0029	-0.0008	0.0783	-15.0	-0.0135	0.0028
9	0.0596	-19.9	0.0029	-0.0630	0.0761	-31.8	-0.0123	-0.0608
10	0.0598	-43.5	0.0027	-0.1253	0.0751	-50.8	-0.0117	-0.1239
11	0.0600	-66.7	0.0026	-0.1877	0.0744	-70.8	-0.0112	-0.1869
12	0.0601	-89.7	0.0025	-0.2501	0.0739	-91.3	-0.0108	-0.2498
13	0.0603	-112.7	0.0024	-0.3125	0.0736	-112.0	-0.0105	-0.3126
14	0.0604	-135.6	0.0022	-0.3749	0.0732	-132.7	-0.0102	-0.3754
15	0.0605	-158.5	0.0021	-0.4373	0.0729	-153.4	-0.0099	-0.4383
16	0.0607	178.6	0.0019	-0.4997	0.0726	-173.8	-0.0096	0.4989

[a] The relative rms residues of the modelling are 6.4×10^{-15} and 3.4×10^{-15}, for $\omega/2\pi = 0.1230$, 0.15625 respectively, which is indicative of 'zero error'.

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References

[1] F. Wehrli. The Origins and Future of Nuclear Magnetic Resonance Imaging. *Physics*

Today 45, pp 34-42, 1992.

[2] S.Y. Kung, K.S. Arun, D.V. Bhaskar Rao. State Space and Singular Value Decomposition-Based Approximation Methods for the Harmonic Retrieval Problem. *J. Amer. Opt. Soc.* **73**, pp 1799-1811, 1983.

[3] W.W.F. Pijnappel, A. van den Boogaart, R. de Beer, D. van Ormondt. SVD-Based Quantification of Magnetic Resonance Signals. *J. Magn. Reson.* **97**, pp 122-134, 1992.

[4] I. Dologlou and G. Carayannis. LPC/SVD Analysis of Signals with Zero-Modelling Error. *Signal Processing* **23**, pp 293-299, 1991.

[5] D.V. Bhaskar Rao and K.S. Arun. Model-Based Processing of Signals : A State Space Approach. *Proc. IEEE*, pp 283-309, 1992.

[6] A.J. van der Veen, E.F. Deprettere, A.L. Swindlehurst. Subspace-Based Signal Analysis Using Singular Value Decomposition. *Proc. IEEE*, pp 1277-1308, 1993.

[7] W.W.F. Pijnappel, R. de Beer, D. van Ormondt. State Space Modelling of Medical NMR Signals. In : J.P. Veen and M.J. de Ket (Eds.), *Proc. ProRISC*, STW, Utrecht, pp 225-230, 1992.

[8] S. Van Huffel, H. Chen, C. Decanniere, P. Van Hecke. Algorithm for Time-Domain NMR Data Fitting Based on Total Least Squares, *J. Magn. Reson.* A110, 1994 (in print).

[9] M. Fiedler. *Special Matrices and their Applications in Numerical Mathematics.* Martinus Nijhoff, Dordrecht, 1986.