Decimative subspace-based parameter estimation techniques applied to magnetic resonance spectroscopy signals

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Abstract— **In this paper, the problem of estimating the frequencies, dampings, amplitudes and phases of closely spaced complex damped exponentials in the presence of noise is considered. In several papers, decimation is proposed as a way to increase the performance of subspace-based parameter estimation methods, in the case of oversampling [1][2][3]. In this paper, a novel extension of the HTLS-method [4] that operates directly on the decimated data matrix is presented, and it is compared to other decimation methods. Experiments on simulated nuclear magnetic resonance (NMR) spectroscopy signals show the influence of decimation on the accuracy and computational complexity of the estimators.**

Keywords— **decimation, subspace-based parameter estimation, NMR, quantitation**

I. Introduction

In various applications of digital signal processing, such as NMR spectroscopy and speech processing, complex damped exponentials are used as a model function. Let $x(t)$ be a sum of K complex damped exponentials, contaminated by additive white noise $n(t)$:

$$x(t) = \sum_{k=1}^{K} c_k z_k^t + n(t), \qquad t = 0, 1, \ldots, N-1 \tag{1}$$

with complex amplitudes $c_k,\ k = 1, \ldots, K$

$$c_k = a_k e^{j(\phi_0 + \phi_k)} \tag{2}$$

and signal poles $z_k,\ k = 1, \ldots, K$

$$z_k = e^{(j2\pi f_k - d_k)/f_{sample}} \tag{3}$$

where a_k represents the amplitude, $(\phi_0 + \phi_k)$ the phase, f_k the frequency and d_k the damping of the kth component, and f_{sample} is the sampling frequency. ϕ_0 is the zero order phase, whereas ϕ_k represents extra degrees of freedom that may be required under certain experimental conditions (usually all ϕ_k are zero). The problem is to estimate these parameters given a set of N noisy data points $x(t),\ \ t = 0, 1, \ldots, N-1$.

It is known that subspace-based parameter estimation techniques perform poorly when applied to a signal consisting of a sum of closely spaced complex damped exponentials [5]. Therefore, in recent publications different decimative approaches were proposed in order to increase the performance of these subspace-based methods. The idea is to artificially increase the frequency separation by decimating (downsampling) the signal, however making sure that no aliasing is introduced.

In this paper a novel extension of the HTLS-method [4] that operates directly on the decimated data-matrix is presented, and it is compared to existing decimative subspace-based algorithms [1][2][3]. Furthermore, the influence of decimation on the accuracy and computational complexity of these subspace-based estimators is analyzed. Extensive Monte-Carlo simulations on simulated NMR signals show the benefits of decimation in the field of NMR spectroscopy.

II. Decimative methods

Three subspace-based methods are briefly described:

- ETLSD: the ESPRIT-Total Least Squares algorithm [6] applied to decimated data, as presented in [1] [2];
- HTLSD: the novel extension of the Hankel-Total Least Squares algorithm [4] for decimated data;
- DESE: another decimative subspace-based parameter estimation algorithm, recently proposed as Decimative Spectral Estimation [3].

In what follows, scalars are represented by lower-case letters, vectors by bold lower case letters and matrices by bold uppercase letters. Furthermore, a Matlab like notation is used: $a(i)$ stands for the ith element of vector $\mathbf{a}$.

A. ETLSD

The approach described in [1] uses several decimated sequences to calculate the sample covariance matrix, which is used to estimate the frequencies and dampings by means of the ESPRIT-TLS method [6].

The original data sequence $\mathbf{x} = [x(0), x(1) \ldots, x(N-1)]$, can be divided into D different decimated sequences $\mathbf{x_i} \in \mathbb{R}^{(N/D)\times 1},\ i = 0, 1, \ldots, D-1$:

$$\mathbf{x_i} = [x(i), x(D+i), \ldots, x((N/D-1)D+i)] \tag{4}$$

with D the decimation factor, which should be chosen such that $|f_k| < (f_{sample})/(2D),\ j = 1, 2, \ldots, K$ in order to avoid aliasing. Using the model (1), we can write:

$$\begin{aligned} x_i(t) &= \sum_{k=1}^{K} c_k z_k^{(Dt+i)} + n(Dt+i),\ t = 0, 1, \ldots, N/D-1 \\ &= \sum_{k=1}^{K} (c_{ki})(z'_k)^t + n(Dt+i) \end{aligned} \tag{5}$$

where $c_{ki} = c_k z_k^i,\ \ k = 1, 2, \ldots, K,\ \ i = 0, 1, \ldots, D-1$ and $z'_k = z_k^D,\ k = 1, 2, \ldots, K$. From each of these decimated sequences a sample covariance matrix with m lags is formed, which can be written as the product of Hankel-matrices:

$$\mathbf{R_i} = \mathbf{X_i} \mathbf{X_i^*} \tag{6}$$

with

$$\mathbf{X_i} = \begin{bmatrix} x_i(0) & x_i(1) & \ldots & x_i(N/D-m) \\ x_i(1) & x_i(2) & \ldots & x_i(N/D-m+1) \\ \vdots & \vdots & \ddots & \vdots \\ x_i(m-1) & x_i(m) & \ldots & x_i(N/D-1) \end{bmatrix}, \tag{7}$$

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where $\mathbf{X_i^*}$ represents the conjugate transpose of $\mathbf{X_i}$. The averaged sample covariance matrix

$$\mathbf{R} = \frac{1}{D}\sum_{i=0}^{D-1}\mathbf{R_i} \tag{8}$$

is then used to estimate the decimated signal poles $z'_k,\ k = 1, 2, \ldots, K$ by means of the ESPRIT-TLS algorithm [6]. From these estimates $\hat{z}'_k$, the estimates of the original poles $\hat{z}_k$, and hence estimates of the frequencies and dampings, are easily obtained. The phases and the amplitudes, contained in c_k, are then calculated as the least squares solution to (1), with z_k replaced by the estimates $\hat{z}_k$.

Since the main computational cost of ETLSD is the eigenvalue decomposition of the $m \times m$ sample covariance matrix $\mathbf{R}$, it is clear that the computational complexity mainly depends on the parameter m.

The method presented in [2] is identical using the same covariance matrix, calculated in a slightly different way.

B. HTLSD

A similar subspace-based method that operates directly on the data matrix is HTLS [4]. The difference between HTLS and ESPRIT-TLS is that HTLS makes use of the singular value decomposition (SVD) of the data matrix instead of the eigendecomposition of the sample covariance matrix.

For noiseless data, using (5), $\mathbf{X_i}$ can be written in terms of Vandermonde matrices:

$$\begin{aligned}\mathbf{X_i} &= \begin{bmatrix} 1 & 1 & \ldots & 1 \\ z'_1 & z'_2 & \ldots & z'_K \\ \vdots & \vdots & \ddots & \vdots \\ {z'_1}^{m-1} & {z'_2}^{m-1} & \ldots & {z'_K}^{m-1} \end{bmatrix} \\ &\quad \begin{bmatrix} c_{1i} & 0 & \ldots & 0 \\ 0 & c_{2i} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & c_{Ki} \end{bmatrix} \begin{bmatrix} 1 & z'_1 & \ldots & {z'_1}^{N/D-m} \\ 1 & z'_2 & \ldots & {z'_2}^{N/D-m} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & z'_K & \ldots & {z'_K}^{N/D-m} \end{bmatrix} \\ &\equiv \mathbf{S C_i T^T}\end{aligned} \tag{9}$$

From this Vandermonde decomposition, the decimated signal poles $z'_k,\ k = 1, \ldots, K$ and complex amplitudes $c_{ki},\ k = 1, \ldots, K$ can immediately be derived. However, no algorithm exists to compute the Vandermonde decomposition directly. Therefore, HTLS makes use of the shift-invariant structure of $\mathbf{S}$ and the singular value decomposition of $\mathbf{X_i}$ to determine the decimated pole estimates $\hat{z}'_k,\ k = 1, 2, \ldots, K$ [4].

From (9) it is clear that the Vandermonde decomposition of every $\mathbf{X_i},\ i = 1, 2, \ldots, D$ has the same (shift-invariant) matrix $\mathbf{S}$, i.e. all decimated sequences have the same poles. Therefore, HTLS can also be applied to the block-Hankel matrix $\mathbf{X}_{stack}$, constructed as follows:

$$\begin{aligned}\mathbf{X}_{stack} &= \begin{bmatrix} \mathbf{X_1} & \mathbf{X_2} & \ldots & \mathbf{X_D} \end{bmatrix} &(10)\\ &= \mathbf{S}\begin{bmatrix} \mathbf{C_1 T} & \mathbf{C_2 T} & \ldots & \mathbf{C_D T} \end{bmatrix}. &(11)\end{aligned}$$

Since in this case all samples are used for the SVD, the estimated poles are more accurate than those estimated from only one decimated sequence.

After the estimation of the signal poles, the phases and the amplitudes are calculated as the least squares solution to (1), with z_k replaced by the estimates $\hat{z}_k$.

Since the main computational cost of HTLSD is the SVD of the $m \times (N + D - mD)$ data matrix $\mathbf{X}_{stack}$, it is clear that the computational complexity, for given N, mainly depends on the parameters m and D.

The fact that HTLS applied to $\mathbf{X}_{stack}$ is the decimative version of HTLS corresponding to ETLSD, can also be deduced from the observation that the averaged sample covariance matrix $\mathbf{R}$ (8) can be written as follows:

$$\mathbf{R} = \frac{1}{D}\begin{bmatrix} \mathbf{X_1} & \mathbf{X_2} & \ldots & \mathbf{X_D} \end{bmatrix} \begin{bmatrix} \mathbf{X_1^*} \\ \mathbf{X_2^*} \\ \vdots \\ \mathbf{X_D^*} \end{bmatrix} = \frac{1}{D}\mathbf{X}_{stack}\mathbf{X}_{stack}^* . \tag{12}$$

C. DESE

This algorithm was presented very recently [3]. Like HTLS, DESE also makes use of the SVD of a Hankel matrix and the full set of data.

A Hankel matrix $\mathbf{X}$ is constructed from the original data sequence (as in (7) with $D = 1$). From this Hankel matrix, $\mathbf{X^D}$ and $\mathbf{X_D}$ are computed by deleting respectively the top and bottom D rows. DESE uses the shift-invariance between $\mathbf{X^D}$ and $\mathbf{X_D}$ in order to estimate the decimated poles.

Without decimation ($D = 1$), this method is identical to a method called MATPEN, proposed in [7].

The main computational cost of DESE consists of the SVD of the $(m-D) \times (N-m+1)$ data matrix $\mathbf{X_D}$ and the eigendecomposition of an $(m-D) \times (m-D)$ matrix. Since D is usually significantly smaller than m, DESE usually requires more operations than ETLSD or HTLSD.

III. Experimental results

Extensive simulations have been performed on typical simulated NMR signals. Below, one representative example simulating a typical 5 peak ^{31}P NMR signal of perfused rat liver, is given. N data points (here, $N = 128$), uniformly sampled at 10 kHz, are generated by a fifth order (K=5) model function (1), of which the parameters are displayed in Table 1. For several combinations of noise level σ_ν, matrix dimension m and decimation factor D, the three described methods are compared by means of Monte-Carlo simulations consisting of 2000 noise realizations each. The data points are perturbed by Gaussian

TABLE I
EXACT PARAMETER VALUES OF THE SIMULATED NMR SIGNAL

peak	f_k(Hz)	d_k(rad/s)	a_k(a.u.)[a]	$\psi_k(^\circ)$[b]
1	-1379	208	6.1	15
2	-685	256	9.9	15
3	-271	197	6.0	15
4	353	117	2.8	15
5	478	808	17.0	15

[a] a.u. means arbitrary units.
[b] $\psi_k = \phi_0 * 180/\pi$ expresses the phase in degrees (in this example $\phi_k = 0,\ k = 1, \ldots, K$).

noise whose real and imaginary components have standard deviation σ_ν. (Relative) root mean squared errors of the estimates of all signal parameters are calculated as well as the percentage of failures per noise level. A failure occurs when not all 5 peaks are resolved within specified intervals lying symmetrically around the exact frequencies, or when the estimated damping is negative. The halfwidths of the intervals are based on Cramer-Rao lower bound considerations, and are respectively 82, 82, 82, 43 and 82 Hz.

The root mean squared error (RMSE) of the frequency estimates (excluding failures) of peak 4 is plotted as a function of σ_ν in Fig. 1, for ETLSD and HTLSD and for different values of m and D. From the curves with $m = 32$ it can be seen that decimation increases the statistical performance significantly, both for ETLSD and HTLSD. There is no significant difference in accuracy between ETLSD and HTLSD. The advantage of HTLSD over ETLSD is that squaring the data, and the associated numerical problems with ill-conditioned matrices, is avoided. Keeping D constant, the accuracy of the frequency estimates increases with increasing m, and hence increasing computational burden (compare the curves with $m = 32,\ D = 1$ to those with $m = 64,\ D = 1$). Comparing the curves with $m = 64,\ D = 1$ to those with $m = 32,\ D = 2$, we see that with a lower m a similar statistical accuracy can be obtained by proportionally increasing D. Simulations with varying m and fixed D show that, for ETLSD and HTLSD, the most accurate estimates are obtained for $m = \frac{N}{2D}$, i.e. for square data matrices $\mathbf{X_i}$. In this case, the statistical accuracy of the estimates obtained with or without decimation is comparable. However, decimation allows to obtain these estimates at a much lower computational cost. Indeed, for $m = \frac{N}{2D}$, the computational complexity is mainly determined by the eigendecomposition of the $(\frac{N}{2D}) \times (\frac{N}{2D})$ matrix $\mathbf{R}$ for ETLSD, and by the SVD of the $(\frac{N}{2D}) \times (\frac{N}{2} + D)$ matrix $\mathbf{X}_{stack}$ for HTLSD. So, for increasing D, the computational cost to obtain the best possible estimates decreases. Therefore, choosing maximal D (in order to avoid aliasing $D < (f_{sample})/(2|f_k|),\ k = 1, \ldots, K$) gives optimal performance, for ETLSD and HTLSD, both in statistical and computational sense.

With $m = \frac{N}{2D}$, the parameter estimates obtained with DESE are much less accurate, as can be seen in Fig. 2. In order to obtain a comparable accuracy with DESE, the matrices $\mathbf{X^D}$ and $\mathbf{X_D}$ should be as square as possible, i.e. $m = \frac{N-D}{2}$. However, since usually $D << N$, increasing D hardly reduces the computational cost because this cost mainly consists of the calculation of the SVD of the $(\frac{N-D}{2}) \times (\frac{N-D}{2})$ matrix $\mathbf{X_D}$ and the eigendecomposition of an $(m-D) \times (m-D)$ matrix. Using $m = \frac{N}{2D}$ on the other hand (as for ETLSD and HTLSD), lowers the computational burden but then the accuracy of the parameter estimates decreases drastically, as shown in Fig. 2.

Some simple tests using the counter of floating points operations (flops) in Matlab illustrate the dependence of the computational complexity of each of the algorithms on D and m , as shown in Table II. Although more effi-

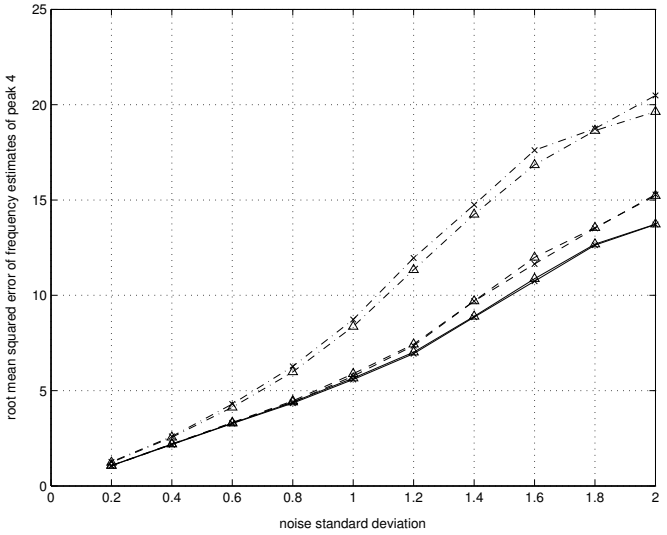

Fig. 1. Plot of RMSE of the frequency estimates of peak 4 versus noise standard deviation σ_ν, for ETLSD (△) and HTLSD (x), for different decimation factors D and matrix dimensions m ($D = 1, m = 32$: dash-dotted line; $D = 1, m = 64$: solid line; $D = 2, m = 32$: dashed line).

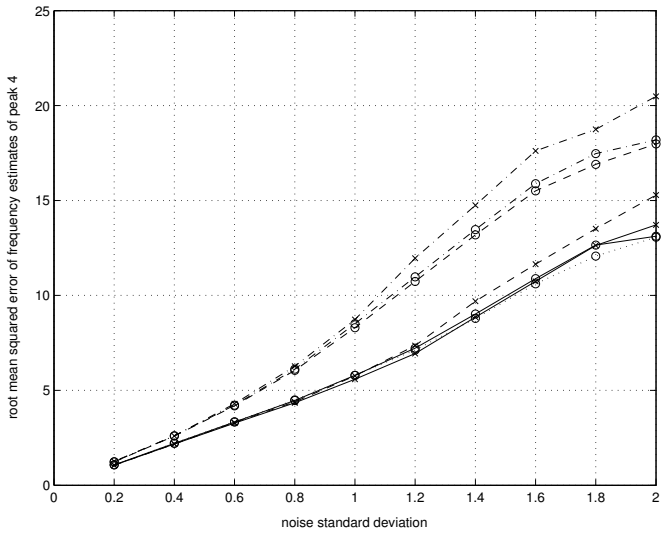

Fig. 2. Plot of RMSE of the frequency estimates of peak 4 versus noise standard deviation σ_ν, for HTLSD (x) and DESE (o), for different decimation factors D and matrix dimensions m ($D = 1, m = 32$: dash-dotted line; $D = 1, m = 64$: solid line; $D = 2, m = 32$: dashed line; $D = 2, m = 64$: dotted line (for DESE only)).

TABLE II

Computational complexity of the algorithms, for different D and m values, expressed as flops/10^6.

D	m	ETLSD	HTLSD	DESE
1	32	3.9	6.8	13.9
2	32	3.6	3.9	13.9
1	64	24.2	12.2	91.1
2	64	n.a.[a]	n.a.[a]	91.0

[a] n.a. means not available: for ETLSD and HTLSD, m must be smaller than N/D.

cient implementations are possible for each algorithm (exploiting the Hankel matrix structure, using partial SVD algorithms), the effect of varying D and/or m on the computational burden will qualitatively be the same as indicated in Table II.

On the other hand, DESE has less failures than HTLSD (and ETLSD, which have a comparable percentage of failures), as shown in Fig. 3. For DESE, the number of failures increases with decreasing D; for ETLSD/HTLSD the number of failures decreases slightly with decreasing D (the differences are small). However, DESE without decimation is still more robust than ETLSD/HTLSD with decimation (for constant m).

IV. Conclusions

In this paper, we presented a decimative extension to the HTLS method [4], and compared it with two other, recently proposed, decimative subspace-based parameter estimation methods: ETLSD [1] [2] and DESE [3]. The principles of the different methods are presented within the same framework, and the relations between the methods are pointed out. The algorithms were tested by means of various Monte-Carlo simulations. It is demonstrated that the dimensions of the data matrix (the number of lags in the covariance matrix) is by far the most important factor determining the statistical accuracy of the parameter estimates, leading to the conclusion that square data matrices give the best parameter estimates. From this observation, it can be derived that decimation as applied in ETLSD and HTLSD, does not lead to better estimates than the best possible ones without decimation. However, decimation allows to obtain estimates with the same accuracy at much lower computational cost. The decimative approach DESE, presented in [3], however, does not have this computational advantage, and its statistical accuracy did not prove to be higher than that of the other two approaches. For very high noise levels the number of failures for DESE seems to be lower than that of ETLSD and HTLSD. It is however not clear how any of these methods can be used in practice (e.g. NMR quantitation) when the percentage of failures of the method is larger than 10%, meaning that one out of ten quantitations is useless.

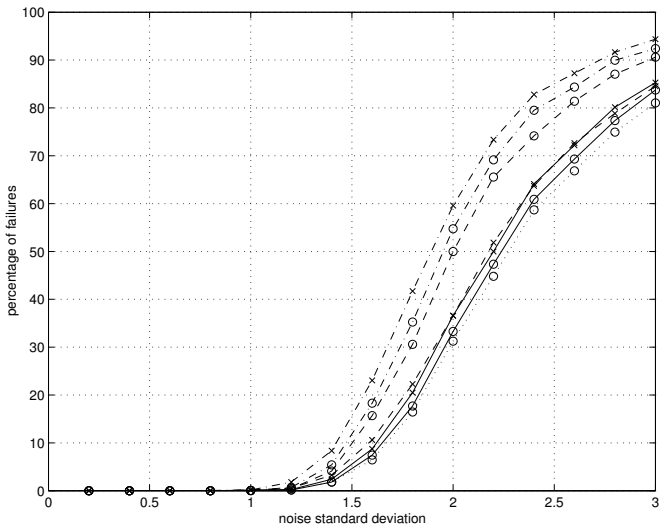

Fig. 3. Plot of percentage of failures versus noise standard deviation σ_ν, for HTLSD (x) and DESE (o), for different decimation factors D and matrix dimensions m ($D=1, m=32$: dash-dotted line; $D=2, m=32$: dashed line; $D=1, m=64$: solid line; $D=2, m=64$: dotted line (for DESE only)).

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