ESTIMATION OF THE PARAMETERS OF TWO-DIMENSIONAL NMR SPECTROSCOPY SIGNALS USING AN ADAPTED SUBBAND DECOMPOSITION

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ABSTRACT

This paper presents a methodology to estimate the parameters of two-dimensional damped/undamped exponentials from high complexity noisy signals, which is the case in 2-D nuclear magnetic resonance spectroscopy signals. The proposed approach performs adaptive subband decomposition combined with a classical frequency estimator based on the Prony model. At each node resulting from the decomposition tree, a stopping rule is computed in order to decide whether the decomposition must be continued or not. The rule is a flatness measure applied on residuals resulting from the estimation step. The method is demonstrated using a simulated signal.

Index Terms— Multidimensional signal processing, magnetic resonance spectroscopy, parameter estimation

1. INTRODUCTION

Since the discovery in 1945 of the nuclear magnetic resonance (NMR) phenomenon, this technique has become a powerful and very successful tool to study structures and molecular interactions [1]. The multidimensional NMR widens the field of investigation to the study of macromolecular structures by allowing the detection and interpretation of interactions that are impossible to analyze along a single dimension (see e.g. [2, 3]).

In this paper, we consider the problem of estimating the parameters of two-dimensional NMR signals modeled as a sum of two-dimensional damped exponentials (also called modes or resonances). For this issue, several high-resolution methods have been developed such as 2-D IQML [4], 2-D MUSIC [5], TLS-Prony [6], Matrix Pencil [7], etc. Nevertheless, whatever the method used, its numerical implementation is problematic. Indeed, in the case of high complexity signals (large number of samples and/or modes), the algorithms have to handle very large matrices that must be inverted and with possible large-order polynomial rooting, resulting in prohibitive computational cost and memory capacity. So, in such cases it would be wiser to perform a subband decomposition before the estimation process itself. This enables one to transform a complex estimation problem into a set of sub-problems, each much simpler and more favorable from a numerical point of view. Moreover, it is known that such decomposition procedures may enhance the performance of the spectral estimator used [8, 9]. The purpose of this work is to present an adaptive subband decomposition scheme combined with a frequency estimator, suitable for the analysis of two-dimensional damped/undamped sinusoidal signals.

The paper is organized as follows. In the next section, the model of a 2-D NMR spectroscopy signal is given, together with an estimation technique. In Section 3, we describe the proposed approach based on an adaptive subband decomposition. This method is then demonstrated in Section 4 by using a simulation signal. Finally, conclusions are given in Section 5.

2. SIGNAL MODELING AND PARAMETER ESTIMATION

The model of the signals considered here is a combination of a certain number I of two-dimensional distinct damped complex exponentials, also called resonances in NMR spectroscopy:

$$d(n,m) = \sum_{i=1}^{I} h_i z_i^n w_i^m + e(n,m), \qquad (1)$$

for $n = 0, ..., N-1$ and $m = 0, ..., M-1$. Here, $z_i = \exp(-\alpha_i^x + j\omega_i^x)$ and $w_i = \exp(-\alpha_i^y + j\omega_i^y)$ are the components of the mode (z_i, w_i) with amplitude h_i ($\alpha_i^x \geq 0$ and $\alpha_i^y \geq 0$). The error term $e(n,m)$ is representative of measurement noise. It is assumed to be a two-dimensional Gaussian complex white noise. The problem is to estimate the number of modes I and the set of parameters $\{z_i, w_i, h_i\}_{i=1}^{I}$, given the noisy measurements $d(n,m)$.

There are several methods that may be used to solve this problem. Most of them are derived from the well known one-dimensional Prony method, which is a linear prediction-based technique. The reader is referred to [10] and references

therein for performance comparison between some of these methods. Without loss of generality, here we choose to use the 2-D TLS-Prony method developed in [6]. The starting point of this method is the following form of equation (1) [6]:

$$d(n,m) = \sum_{k=1}^{K} \sum_{l=1}^{L_k} a_{k,l} p_{x_k}^n p_{y_{k,l}}^m + e(n,m) \tag{2}$$

$$= \sum_{k=1}^{K} c_{k,m} p_{x_k}^n + e(n,m), \tag{3}$$

where

$$c_{k,m} = \sum_{l=1}^{L_k} a_{k,l} p_{y_{k,l}}^m, \tag{4}$$

p_{x_k} is the kth x-mode (x-component of 2-D exponential), $p_{y_{k,l}}$ is the k,lth y-mode, $a_{k,l}$ is the k,lth amplitude coefficient and L_k is the number of y-modes corresponding to the kth x-mode. In order to estimate the 2-D signal parameters, the idea is to perform a set of 1-D estimation procedures using (3) and (4). Indeed, it is clear from (3) that the sequence obtained for a fixed value of m is a 1-D exponential signal whose parameters may be estimated with a 1-D method.

Generally speaking, use of the so-called high-resolution techniques to estimate the parameters of a 2-D signal leads to good performances in terms of precision and resolution, as compared to that obtained with the classical Fourier transform. Unfortunately, when the number of measurements and/or the number of signal parameters are large, it is often difficult to take advantage of their performance because of implementation problems. For instance, the dimension of the linear system involved to obtain the parameters p_{x_k} in (3) is approximately $NM \times p$, where $p \geq K$ is known as the prediction order. So it is clear that, in this case, it is necessary to reduce the underlaying problem complexity by using some separation techniques such as subband decomposition.

3. SUBBAND DECOMPOSITION

The concept of subband decomposition is used in various fields of investigation. In the particular domain of spectral analysis, the advantages of a subband decomposition approach, have been emphasized by several authors [9, 11–13]. This idea enables one to transform a complex estimation problem into a set of sub-problems, each being much simpler than the original.

The decomposition is achieved classically through filtering and decimation stages, but the question remains of how to perform the decomposition properly. In particular, a question that arises is the endpoint of the decomposition. At first, a tradeoff must be reached between two alternatives. To improve frequency resolution, it is necessary to increase the decimation factor, but the number of data samples reduces as the decimation gets deeper. Secondly, it would be desirable to stop the decomposition as soon as all the information is retrieved. These remarks suggest using adaptive forms of decomposition rather than simple uniform ones. In this case, the decimation is carried out according to the spectral content of the subbands encountered, but the problem is then to establish a stopping rule that determines an optimal decomposition tree (in some sense).

For instance, in [14], the selection of the optimal decomposition is made by maximizing the number of modes over the whole decomposition tree. The number of modes lying in some band being unknown, it has to be estimated using, say, the minimum description length (MDL) criterion [15]. The problem that arises with such an approach is that it does not allow to stop the decomposition of empty bands or those where the modes can easily be retrieved. As an alternative, we propose to use a stop criterion that reflects the quality of the estimation in a given subband, that is, a measure of whiteness of the corresponding residuals. Unlike adaptive decompositions using order criteria, the decision about stopping or following up the decomposition is made after the estimation process. This allows one to minimize the number of possible missed components.

3.1. Decomposition of a 2-D Signal

The subband decomposition is achieved by successive filtering and decimation stages as illustrated in Fig. 1. In each subband (node), the model of the 2-D signal is still a sum of a (reduced) number of modes which can be estimated by the TLS-Prony method presented in the previous section.

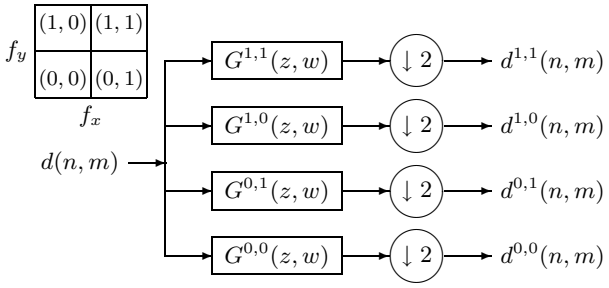

Fig. 1. Principle of decomposition of a 2-D signal $d(n,m)$ into four subbands. $G^{i,k}(z,w)$ are the frequency responses of bandpass filters.

Let $d'(n,m)$ be the sub-signal corresponding to a given node in the decomposition tree, constituted of I' 2-D damped exponentials:

$$d'(n,m) = \sum_{i=1}^{I'} h'_i z_i'^n w_i'^m + e'(n,m). \tag{5}$$

Assume that $\hat{I}'$ modes $(\hat{z}_i, \hat{w}'_i)$ are detected and estimated by the TLS-Prony approach with amplitudes $\hat{h}'_i$, and define the

estimation residuals by the difference between the true subsignal and the reconstructed one:

$$r(n,m) = d'(n,m) - \sum_{i=1}^{\hat{I}'} \hat{h}'_i \hat{z}'^n_i \hat{w}'^m_i. \quad (6)$$

for $n = 0, ..., N'-1$ and $m = 0, ..., M'-1$. Ideally, if all subsignal modes have been correctly retrieved, the residuals are close to white noise. If one or more modes are missed, then the signal $r(n,m)$ still contains information. The stopping rule described below is based on this aspect.

3.2. A Measure of Spectral Flatness

The stopping rule of the decomposition tests for the presence of some "periodic" component in the residual signal $r(n,m)$. For that, several statistics may be considered, such as Fisher's g-statistic [16], Drouiche's test for whiteness [17], etc. Here we use the Drouiche's measure which is developed for 1-D sequences.

If we denote by $\hat{Q}(\omega)$ the periodogram of a 1-D Gaussian sequence of length L, then the measure of spectral flatness (whiteness) is defined by:

$$\hat{W} = \log \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{Q}(\omega) d\omega - \frac{1}{2\pi} \int_{-\pi}^{\pi} \log \hat{Q}(\omega) d\omega - \gamma, \quad (7)$$

where $\gamma = 0.57721$ denotes the Euler constant. It can be shown that $\hat{W} \approx 0$ for a white noise and $\hat{W} \to \infty$ if the sequence is maximally correlated [17]. In practice, we reject the whiteness hypothesis if $\hat{W} > t_\alpha$, where t_α is a threshold obtained using a significance level α:

$$t_\alpha = \frac{\sqrt{2}\nu_0}{\sqrt{L}} \mathrm{erf}^{-1}(1-2\alpha), \quad (8)$$

where $\nu_0 = \sqrt{\pi^2/6 - 1}$, and $\mathrm{erf}^{-1}(x)$ is the inverse of the standard error function

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \quad (9)$$

In order to test for the whiteness of the 2-D signal $r(n,m)$, we should first compute its periodogram defined by:

$$\hat{P}'(\omega_1, \omega_2) = \frac{1}{N'M'} \left| \sum_{n=0}^{N'-1} \sum_{m=0}^{M'-1} r(n,m) e^{-jn\omega_1} e^{-jm\omega_2} \right|^2. \quad (10)$$

Then, we apply the previous measure (7) on the two marginals of $\hat{P}'(\omega_1, \omega_2)$ along the two dimensions to obtain $\hat{W}_1$ and $\hat{W}_2$. The signal $r(n,m)$ is a white noise only if the two measures are less than the threshold t_α.

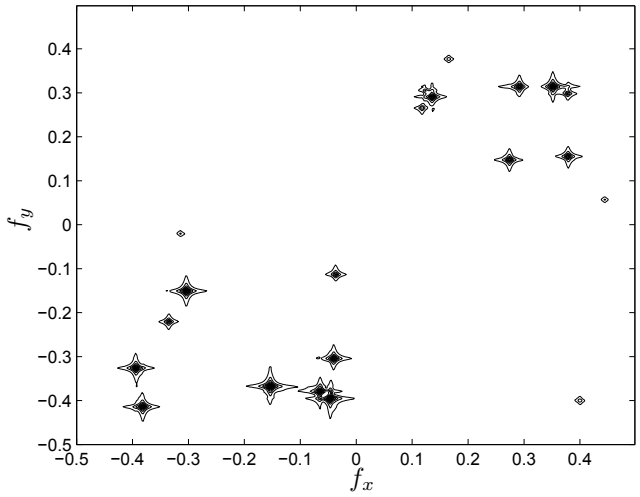

Fig. 2. Power spectrum of the noise-free simulated signal.

4. EXPERIMENTS

The simulation signal is intended to demonstrate the capability of the proposed approach to track the spectral subbands in which information is localized. The signal contains 21 modes. Ten modes are positioned randomly in the lower-left quarter of the frequency plane (i.e. in the frequency range $[-.5, 0] \times [-.5, 0]$), and ten other modes in the upper-right quarter. The last one is located at $(.4, -.4)$. All damping factors are equal to 0.02 and the amplitudes are generated randomly in the interval $[0.5, 3.5]$. The variance of the additive noise is fixed to 10^{-4}. The generated samples form a data matrix of dimension 256×256, whose Fourier transform is shown in Fig. 2.

The results obtained with a prediction order $p = 6$, for the estimation procedure, and a significance level $\alpha = 5\%$ are shown in Fig. 3. One can observe in Fig. 3(a) that the decomposition is generally deeper in the spectral regions where several modes are located. On the other hand, for remote modes, the decomposition is stopped at an early level. This is the case for instance with mode $(.4, .4)$. So the method is able to adapt itself to the local complexity of a signal, allowing one to reduce the calculation time, as compared to a uniform decomposition in which several small subbands need to be analyzed. Moreover, all the modes have been detected. For example, Figs. 3(b) and 3(c) shows two closely spaced modes (appearing in distinct subbands) that are correctly estimated.

5. CONCLUSION

In this paper, we have proposed an adapted subband decomposition approach for the analysis of 2-D NMR data. This method uses a stopping rule based on a spectral flatness measure of the subband residuals. If the test for whiteness fails in a given node, then the decomposition is carried on; other-

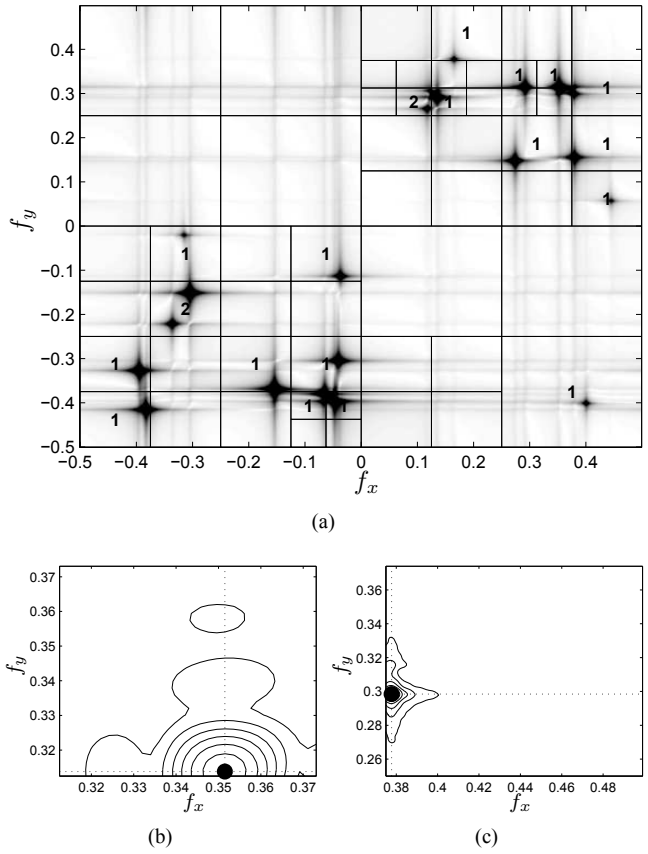

Fig. 3. Some results achieved on the simulated signal. (a) Representation of the noisy signal with the final spectral subbands and the number of estimated modes. Reconstructed contour plot in (b) band $[.375, .5] \times [.25, .375]$ and (c) band $[.3125, .375] \times [.3125, .375]$.

wise the decomposition is stopped. The results obtained point out the advantages of the method over global estimation with uniform decomposition. Application on real data will be presented in future work.

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