DMUSIC Algorithm for 2D NMR Signals

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Abstract— In this paper, we will propose a super-resolution scheme for the parameter estimation of two-dimensional (2-D) NMR signals. 2-D NMR signals can be modeled as the summation of 2-D damped sinusoids. The frequencies and the damping factors of 2-D damped sinusoids play important roles in protein structure determination using 2-D NMR spectroscopy. We will develop a super-resolution frequency and damping factor estimation algorithm—damped MUSIC (DMUSIC) algorithm. Since the DMUSIC algorithm makes full use of the rank-deficiency and the Hankel property of the data matrix composed of the 2-D NMR data, compared with other NMR data analysis algorithms, it can resolve the NMR spectroscopy under low signal to noise ratio. The performance of the DMUSIC algorithm is demonstrated by simulations.

Key words: 2D NMR Signal, DMUSIC algorithm

I. INTRODUCTION

The spectral analysis of the NMR spectroscopy is very important in protein structure determination.

We will develop a super-resolution algorithm for 2-D NMR signals in this paper, which is called 2-D DMUSIC algorithm because it has super-resolution like the MUSIC algorithm [1].

Discrete two-dimensional (2-D) NMR signals can be expressed as two-dimensional time-series $\{x(n,m)\}$ [2]

$$x(n,m) = \sum_{k=1}^{K} c_k e^{s_k^{(1)}n + s_k^{(2)}m}, \qquad (1)$$

where $s_k^{(l)} = -\alpha_k^{(l)} + j\omega_k^{(l)}$, and $\omega_k^{(l)} \in [-\pi, \pi]$, $\alpha_k^{(l)} \in \mathcal{R}^+$, which is called the damping factor. Without loss of generality, we suppose that $s_k = (s_k^{(1)}, s_k^{(2)})$ be distinct. If the measurement error or noise $w(n,m)$ is considered, the measured NMR data can be expressed as

$$y(n,m) = x(n,m) + w(n,m), \qquad (2)$$

for $n = 0, 1, \cdots, N-1$ and $m = 0, 1, \cdots, M-1$. In the above expression N and M are acquisition time of each time domain. Normally, we have to make sure $N, M \geq 2K$. We will further assume $N = M$ in this paper.

To determine the protein structure by means of the 2-D NMR spectroscopy, the complex frequencies s_k of NMR

data have to be estimated from $y(n,m)$. In [3], we have developed the 1-D DMUSIC algorithm–a parameter estimation algorithm for 1-D damped sinusoids, which can be used for 1-D NMR signals. Based on the 1-D DMUSIC algorithm, we derive a 2-D MUSIC algorithm for 2-D NMR signals.

II. 2-D DMUSIC ALGORITHM

To obtain 2-D MUSIC algorithm for the 2-D NMR signal modeled in (1) and (2), we first generate an $(N-L+1) \times L$ matrix,

$$\mathbf{A}(l) = \begin{pmatrix} y(l,0) & \cdots & y(l,L-1) \\ y(l,1) & \cdots & y(l,L) \\ \vdots & \vdots & \vdots \\ y(l,N-L) & \cdots & y(l,N-1) \end{pmatrix}, \qquad (3)$$

for $l = 1, 2, \cdots, N-1$. Using $\mathbf{A}(l)$, an $(N-L+1)L \times (N-L+1)L$ matrix is formed,

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}(0) & \mathbf{A}(1) & \cdots & \mathbf{A}(N-L) \\ \mathbf{A}(1) & \mathbf{A}(2) & \cdots & \mathbf{A}(N-L+1) \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{A}(L-1) & \mathbf{A}(L) & \cdots & \mathbf{A}(N-1) \end{pmatrix}. \qquad (4)$$

L must satisfied $2K \leq L \leq N - 2K$. It is usually $\lceil N/2 \rceil$ to obtain the best performance.

If we define the $\mathbf{r}(\mathbf{s}_k)$ as following

$$\mathbf{r}(\mathbf{s}_k) = \begin{pmatrix} 1 \\ e^{s_k^{(2)}} \\ \vdots \\ e^{(L-1)s_k^{(2)}} \\ e^{s_k^{(1)}} \\ e^{s_k^{(1)}+s_k^{(2)}} \\ \vdots \\ e^{s_k^{(1)}+(L-1)s_k^{(2)}} \\ \vdots \\ e^{(N-L)s_k^{(1)}} \\ e^{(N-L)s_k^{(1)}+s_k^{(2)}} \\ \vdots \\ e^{(N-L)s_k^{(1)}+(L-1)s_k^{(2)}} \end{pmatrix}, \quad \bar{\mathbf{r}} = \frac{\mathbf{r}}{\|\mathbf{r}\|}, \qquad (5)$$

then s_k can be estimated by finding the peaks of the following spectrum

$$\frac{1}{\bar{\mathbf{r}}^H(\mathbf{s}) \sum_{n=K+1}^{(N-L+1)L} \mathbf{v}_n^* \mathbf{v}_n^T \bar{\mathbf{r}}(\mathbf{s})}, \tag{6}$$

where $\mathbf{v}_n$ for $n = K+1, \cdots, (N-L+1)L$ are right eigenvector of $\mathbf{A}$.

The algorithm discussed above not only looks like but also performs as well as MUSIC algorithm when applied to pure sinusoidal frequency estimation. It is, therefore, called the *2-D damped MUSIC* (2-D MUSIC) algorithm. However, there is a crucial difference between the MUSIC algorithm and DMUSIC algorithm. The MUSIC algorithm is for stationary signal (or pure sinusoidal signals), where the correlation matrix of the signal is available. The 2-D DMUSIC algorithm, on the other hand, is for two-dimensional nonstationary signal, such as 2-D NMR signal, which directly exploit the structure of the data matrix.

III. COMPUTER SIMULATION EXAMPLE

To illustrate the theoretical consistency, the 2-D DMUSIC algorithm is tested by a set of real NMR data obtained from National Institute for Health. The length of the data is 12×12. The 2-D FFT of NMR data zero padded upto 512 points is shown in Figure 1. From the figure, it is very difficult to estimate the frequencies of the NMR data. If 2-D DMUSIC algorithm ($N = 12, L = 6$) is used to estimate the parameters of the NMR data, the 2-D DMUSIC spectrum $P(0,0; \omega^{(1)}, \omega^{(2)})$ and its contour are shown in Figure 2. From the figure, $P(0,0; \omega^{(1)}, \omega^{(2)})$ have five peaks. The 2-D spectrum $P(\alpha^{(1)}, \alpha^{(2)}; 0.10\pi, -0.12\pi)$ and its contour are shown in Figure 3. The estimated the frequencies and the damping factors of the NMR signal are shown in Table I.

IV. DISCUSSION

This paper develops a super-resolution parameter estimation algorithm–DMUSIC for 2-D NMR signals. Although the MUSIC analysis is applied to 1-D NMR in [4], the damping factors of NMR signals are ignored there. Our 2-D DMUSIC algorithm not only can estimate the frequencies and the damping factors of the NMR signals simultaneously but also can be easily extended to the parameter estimation of M-D NMR signals.

TABLE I
ESTIMATED FREQUENCIES AND DAMPING FACTORS

k	$\alpha_k^{(1)}$	$\omega_k^{(1)}$	$\alpha^{(2)}{}_k$	$\omega_k^{(2)}$
1	0.06	0.04π	0.06	-0.02π
2	0.07	-0.56π	0.08	0.10π
3	0.07	-0.42π	0.09	0.40π
4	0.13	0.10π	0.09	-0.12π
5	0.21	0.12π	0.29	0.64π

REFERENCES

[1] S. Haykin, *Adaptive Filter Theory*, Prentice Hall, 1991.
[2] A. Bax, "A simple description of two-dimensional NMR spectroscopy," *Bulletin of Magnetic Resonance* vol.7, pp. 167–183, 1985.
[3] Y. Li, K. J. R. Liu, J. Razavilar, "Improved parameter estimation schemes for damped sinusoidal signals," *Technical Report of SRC of University of Maryland*, T.R. 95-11, 1995.
[4] S. A. Meyer, D. L. Orth, M. A. Morgenstern, and D. W.Noid, "MUSIC analysis applied to NMR," *Journal of Magnetic Resonance* vol.86, pp. 406–409, 1990.

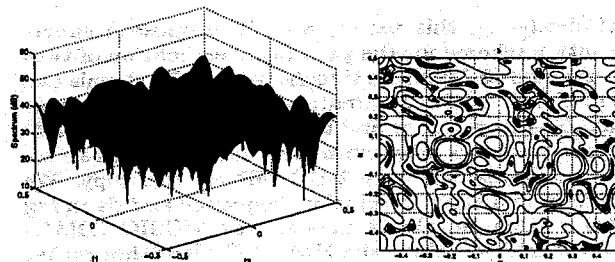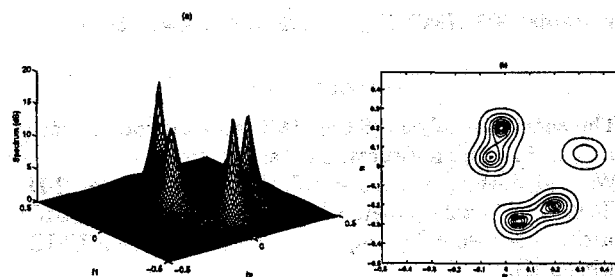Fig. 1. 2-D FFT of NMR data zero padded upto 512, (a) Fourier spectrum, and (b) its contour.

Fig. 2. The spectrum $P(0,0; \omega^{(1)}, \omega^{(2)})$ and its contour for 2-D NMR signal.
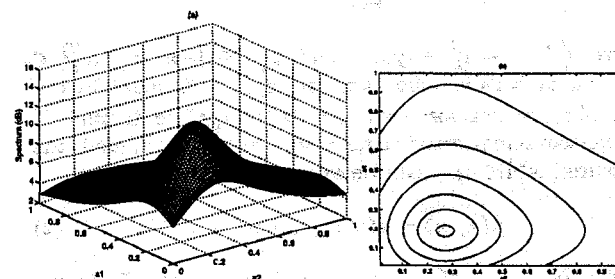

Fig. 3. The spectrum $P(\alpha^{(1)}, \alpha^{(2)}; 0.10\pi, -0.12\pi)$ and its contour for 2-D NMR signal.