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Correcting for Phase Distortion of NMR Spectra Analyzed Using Singular-Value Decomposition of Hankel Matrices

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In a series of papers [e.g. (*1–3*)], it was suggested that methods based on singular-value decomposition techniques of Hankel matrices could be used to analyze data in NMR experiments. We will review the basic idea behind this method from a general point of view. By means of an example we will show that the method can lead to poorly phased spectra, despite the fact that the Fourier transform of the unprocessed data leads to a well-phased, albeit noise-corrupted, spectrum. It is then shown that the general scheme can be modified in a way that such problems will be reduced. It follows from results in the area of stochastic realization theory and stochastic model reduction that, in the infinite-data case, the processed data are always correctly phased if the proposed modification of the method is used. By means of an example it is shown that this can also be expected in the finite-data case. This new methodology could be useful for the improvement of the quality of NMR spectra, particularly for the avoidance of the introduction of phasing problems that might arise during automated processing using the current Hankel-matrix-based methods.

The basic idea of the Hankel-matrix-based method is as follows. Let a sampled free induction decay be given as

$$\mathrm{FID}(n) = \sum_{j=1}^{k} c_j e^{(2\pi i\omega_j - d_j)(n-1)\Delta T} + \epsilon((n-1)\Delta T),$$
$$n = 1, 2, \ldots,$$

where $\omega_j \in [0, 1/\Delta T]$ is the frequency of the jth component of the signal, d_j is the corresponding damping factor, ΔT is the sampling interval, $[\epsilon(\Delta T(n-1))]_{n\geq 1}$ is the noise sequence, and c_j are the coefficients that are weighting the frequency components.

The coefficients of the FID are then placed in the Hankel matrix

$$\mathbf{H} = \begin{bmatrix} \mathrm{FID}(1) & \mathrm{FID}(2) & \mathrm{FID}(3) & \mathrm{FID}(4) & \cdots \\ \mathrm{FID}(2) & \mathrm{FID}(3) & \mathrm{FID}(4) & \cdots & \cdots \\ \mathrm{FID}(3) & \mathrm{FID}(4) & & & \\ \mathrm{FID}(4) & \vdots & & & \\ \vdots & \vdots & & & \end{bmatrix}.$$

If $\mathbf{H} \approx \mathcal{O}_k \mathcal{R}_k$ is an approximate factorization of the Hankel matrix $\mathbf{H}$ such that the finite matrices $\mathcal{O}_k$ and $\mathcal{R}_k$ are of full rank k, then we set $\mathbf{A}_k$ such that $\mathcal{O}_k^{\mathrm{down}}\mathbf{A}_k = \mathcal{O}_k^{\mathrm{up}}$, $\mathbf{B}_k$ as the first column of $\mathcal{R}_k$, and $\mathbf{C}_k$ as the first row of $\mathcal{O}_k$. Here $\mathcal{O}_k^{\mathrm{up}}$ is the matrix obtained from $\mathcal{O}_k$ by deleting the first row and $\mathcal{O}_k^{\mathrm{down}}$ is the matrix obtained from $\mathcal{O}_k$ by deleting the last row. Clearly, the identity $\mathcal{O}_k^{\mathrm{down}}\mathbf{A}_k = \mathcal{O}_k^{\mathrm{up}}$ can in practice not be expected to be precise and an approximate solution must be found.

Given the matrices $(\mathbf{A}_k, \mathbf{B}_k, \mathbf{C}_k)$, the FID is then assumed to be modeled by

$$\mathrm{FID}(n) \approx \mathbf{C}_k \mathbf{A}_k^{n-1} \mathbf{B}_k, \quad n = 1, 2, \ldots.$$

If the matrix $\mathbf{A}_k$ is diagonalized, i.e., if for some invertible $\mathbf{T}$, $\mathbf{T}\mathbf{A}_k\mathbf{T}^{-1} =: \mathrm{diag}(\alpha_1, \ldots, \alpha_k) =: d\mathbf{A}_k$, then with $d\mathbf{B}_k := \mathbf{T}\mathbf{B}_k$, $d\mathbf{C}_k := \mathbf{C}_k\mathbf{T}^{-1}$,

$$\mathrm{FID}(n) \approx d\mathbf{C}_k d\mathbf{A}_k^{n-1} d\mathbf{B}_k = \sum_{j=1}^{k} \gamma_j \beta_j \alpha_j^{n-1},$$
$$n = 1, 2, \ldots,$$

where $d\mathbf{B}_k = (\beta_1 \cdots \beta_k)^{\mathrm{T}}$, $d\mathbf{C}_k = (\gamma_1 \cdots \gamma_k)$. Hence we set $\hat{c}_j := \gamma_j\beta_j$, $j = 1, \ldots, k$.

As $\alpha_j \approx e^{(2\pi i\omega_j - d_j)\Delta T}$, $j = 1, 2, \ldots, k$, we set $\hat{d}_j = -\log|\alpha_j|/\Delta T$, $\hat{\omega}_j = \mathrm{angle}(\alpha_j)/2\pi\Delta T$, $j = 1, 2, \ldots, k$. The typical implementation of the scheme is as follows. Let

$$\mathbf{H}_N = \begin{bmatrix} \mathrm{FID}(1) & \mathrm{FID}(2) & \mathrm{FID}(3) & \cdots & \mathrm{FID}(N) \\ \mathrm{FID}(2) & \mathrm{FID}(3) & \cdots & \cdots & \mathrm{FID}(N+1) \\ \mathrm{FID}(3) & \vdots & & & \vdots \\ \vdots & \vdots & & & \vdots \\ \mathrm{FID}(N) & \mathrm{FID}(N+1) & \cdots & \mathrm{FID}(2N) & \mathrm{FID}(2N+1) \end{bmatrix},$$

where N is generally chosen as a compromise such that $\mathbf{H}_N$ provides a "good" approximant of the semi-infinite Hankel matrix $\mathbf{H}$ and $\mathbf{H}_N$ is not too large for reasonable computational speed. Then a singular-value decomposition is performed, $\mathbf{H}_N = \mathbf{U\Sigma V}$, where $\mathbf{\Sigma} = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_l) \in \mathcal{C}^{l \times l}$, $\sigma_1 \geq \sigma_2$

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$\geqslant \cdots \geqslant \sigma_l > 0$, is diagonal with strictly positive entries, $\mathbf{U} \in \mathcal{C}^{N \times l}$ such that $\mathbf{U}^*\mathbf{U} = \mathbf{I}_l$, $\mathbf{V} \in \mathcal{C}^{l \times N}$, $\mathbf{V}\mathbf{V}^* = \mathbf{I}_l$. Note that if the measurements of the FID were not corrupted by noise then the dimension of $\mathbf{\Sigma}$ would equal the number of frequency components in the signal; i.e., $l = k$ if $N \geqslant k = \text{rank}(\mathbf{H})$ (Kronecker's theorem). Due to the presence of noise we typically have that $l \geqslant k$.

In order to account for the noise in the signal we use the following heuristic. The noise level is considered to be "low" with respect to the signal. It is then argued that the small singular values $\sigma_{k+1}, \ldots, \sigma_l$ are due to the noise and the larger singular values are due to the signal. Therefore the small singular values are truncated away and only the following reduced matrices are considered: $\mathbf{\Sigma}_k = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k)$, $\mathbf{V}_k$ the first k rows of $\mathbf{V}$, and $\mathbf{U}_k$ the first k columns of $\mathbf{U}$. We then set $\mathcal{O}_k = \mathbf{U}_k\mathbf{\Sigma}_k^{1/2}$, $\mathcal{R}_k^{1/2} = \mathbf{\Sigma}^{1/2}\mathbf{V}_k$ and apply the above described method to estimate the parameters of the signal from $\mathcal{O}_k$ and $\mathcal{R}_k$.

In the following example, we demonstrate a possible problem with this method. We give an example of an FID that is phased; i.e., the real part of the Fourier transform of the signal is positive. But the real part of the Fourier transform obtained from the simulated FID using the estimated parameters $\hat{\omega}_k$, $\hat{R}_k$, $\hat{c}_k$ is no longer positive. This might lead to problems in the interpretation of spectra that have been processed using this method. This problem arises due to a fundamental shortcoming of the approximation step in which $\mathbf{\Sigma}$, $\mathbf{V}$, $\mathbf{U}$ are replaced by $\mathbf{\Sigma}_k$, $\mathbf{V}_k$, $\mathbf{U}_k$. Such problems were previously recognized in the econometrics literature (*4*), where related Hankel based methods are used to analyze time-series data.

Figure 1a shows the real part of the Fourier transform of a simulated FID with noise added. In Fig. 1b, the Fourier transform is shown of an FID that was calculated based on the estimates obtained using the method discussed above. While the unprocessed Fourier transform is well phased, the phasing is completely destroyed by the estimation technique.

We now introduce a modification of the previously described method to ensure that proper phasing is preserved by the data-processing method. In this context, functions of positive type play an important role. A rational function

$$F(z) = \sum_{n=-\infty}^{\infty} f_n z^n, \quad |z| = 1,$$

is said to be of *positive type* if $F(z) \geqslant 0$, $|z| = 1$. The application of this definition to NMR is as follows. Let $[\text{FID}(n)]_{n \geqslant 1}$ be the sampled FID of an NMR experiment, with sampling interval ΔT. Let

$$\text{DFT}(\omega) = \sum_{j=1}^{\infty} \text{FID}(j) e^{-2\pi i \omega \Delta T(j-1)}, \quad \omega \in \left[0, \frac{1}{\Delta T}\right]$$

be the discrete Fourier transform (DFT) of the FID. In many experiments the FID is such that the DFT is *positive real*, i.e., has positive real part,

$$\begin{aligned} \text{Real}[\text{DFT}(\omega)] &= \frac{1}{2}\Big[\sum_{j=1}^{\infty} \text{FID}(j) e^{-2\pi i \omega \Delta T(j-1)} \\ &\quad + \sum_{j=1}^{\infty} \overline{\text{FID}(j)}\, e^{2\pi i \omega \Delta T(j-1)}\Big] \\ &= \frac{1}{2}\Big[\text{FID}(1) + \overline{\text{FID}(1)} \\ &\quad + \sum_{j=2}^{\infty} \text{FID}(j) e^{-2\pi i \omega \Delta T(j-1)} \\ &\quad + \sum_{j=2}^{\infty} \overline{\text{FID}(j)}\, e^{2\pi i \omega \Delta T(j-1)}\Big] \geqslant 0, \end{aligned}$$

for all $\omega \in [0, 1/\Delta T]$. Note that typically FID(1) is real and hence

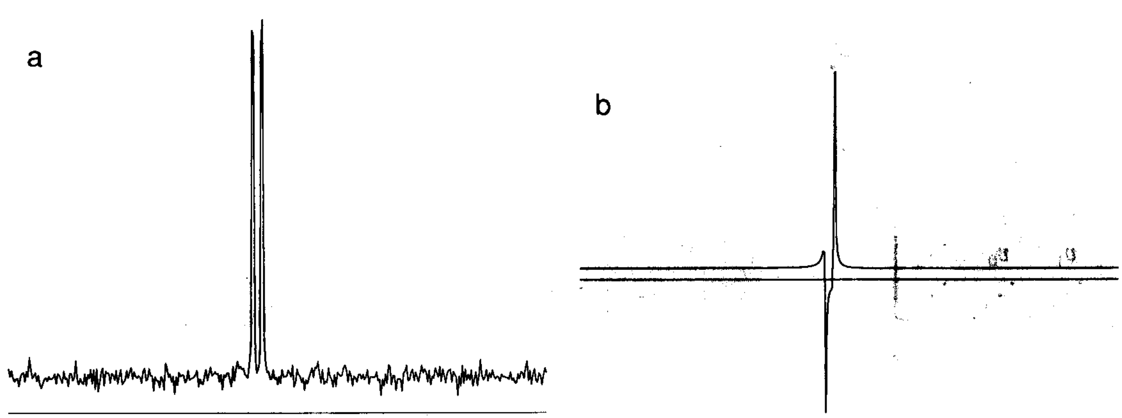

FIG. 1. (a) Real part of DFT of noisy FID. (b) Spectrum after processing with the "standard" Hankel-matrix-based method ($k = 2$).

$$2\text{Real}[\text{DFT}(\omega)] = 2\text{FID}(1) + \sum_{j=2}^{\infty} \text{FID}(j)e^{-2\pi i\omega\Delta T(j-1)} + \sum_{j=2}^{\infty} \overline{\text{FID}(j)}\, e^{2\pi i\omega\Delta T(j-1)}.$$

Now set $f_0 := 2\text{FID}(1)$; $f_n := \overline{\text{FID}(n)}$, $n \geqslant 1$; $f_n := \text{FID}(n)$, $n \leqslant -1$; and $F(z) = \sum_{n=-\infty}^{\infty} f_n z^n$, $|z| = 1$. Then for $z = e^{2\pi i\omega\Delta T}$ and $\omega \in [0, 1/\Delta T]$, $F(z) = 2\text{Real}[\text{DFT}(\omega)]$. This shows that F is of positive type if $\text{DFT}(\omega) \geqslant 0$ for all $\omega \in [0, 1/\Delta T]$.

Now let

$$\mathbf{H_F} = \begin{bmatrix} f_{-1} & f_{-2} & f_{-3} & f_{-4} & \cdots \\ f_{-2} & f_{-3} & f_{-4} & \cdots & \cdots \\ f_{-3} & f_{-4} & & & \\ f_{-4} & \vdots & & & \\ \vdots & \vdots & & & \end{bmatrix} = \begin{bmatrix} \text{FID}(2) & \text{FID}(3) & \text{FID}(4) & \text{FID}(5) & \cdots \\ \text{FID}(3) & \text{FID}(4) & \text{FID}(5) & \cdots & \cdots \\ \text{FID}(4) & \text{FID}(5) & & & \\ \text{FID}(5) & \vdots & & & \\ \vdots & \vdots & & & \end{bmatrix}$$

be a semi-infinite Hankel matrix. Note the slight modification of the definition of the Hankel matrix. Under the assumption that F is of positive type, it can be shown (5) that a factorization $\mathbf{T}_F = \mathbf{T}_v^*\mathbf{T}_v$ exists for

$$\mathbf{T}_F = \begin{bmatrix} f_0 & f_{-1} & f_{-2} & \cdots & \cdots \\ f_1 & f_0 & f_{-1} & \ddots & \cdots \\ f_2 & f_1 & f_0 & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} = \begin{bmatrix} 2\text{FID}(1) & \text{FID}(2) & \text{FID}(3) & \cdots & \cdots \\ \overline{\text{FID}(2)} & 2\text{FID}(1) & \text{FID}(2) & \cdots & \cdots \\ \overline{\text{FID}(3)} & \overline{\text{FID}(2)} & 2\text{FID}(1) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

and

$$\mathbf{T}_v = \begin{bmatrix} v_0 & 0 & 0 & \cdots \\ v_1 & v_0 & 0 & \ddots \\ v_2 & v_1 & v_0 & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{bmatrix}$$

for some $v_0 > 0$ and $v_i \in \mathcal{C}$, $i = 1, 2, \ldots$. By analogy with stochastic realization theory (6) we call $(\mathbf{T}_v^{\mathrm{T}})^{-1}\mathbf{H}_F\mathbf{T}_v^{-1}$ the *canonical correlation operator*. In practical situations we must work with finite approximations of these semi-infinite matrices. Therefore the n-dimensional approximant $\mathbf{T}_N$ of $\mathbf{T}_F$,

$$\mathbf{T_N} = \begin{bmatrix} f_0 & f_{-1} & f_{-2} & \cdots & f_{1-n} \\ f_1 & f_0 & f_{-1} & \cdots & f_{2-n} \\ f_2 & f_1 & f_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & f_{-1} \\ f_{n-1} & \cdots & \cdots & f_1 & f_0 \end{bmatrix} = \begin{bmatrix} 2\text{FID}(1) & \text{FID}(2) & \text{FID}(3) & \cdots & \text{FID}(n) \\ \overline{\text{FID}(2)} & 2\text{FID}(1) & \text{FID}(2) & \cdots & \text{FID}(n-1) \\ \overline{\text{FID}(3)} & \overline{\text{FID}(2)} & 2\text{FID}(1) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \text{FID}(2) \\ \overline{\text{FID}(n)} & \cdots & \cdots & \overline{\text{FID}(2)} & 2\text{FID}(1) \end{bmatrix},$$

and the Cholesky factorization $\mathbf{T}_N = \mathbf{L}^*\mathbf{L}$, is formed, where $\mathbf{L}$ is a lower triangular $N \times N$ matrix with positive diagonal. Now set

$$\mathbf{H_N} = \begin{bmatrix} \text{FID}(2) & \text{FID}(3) & \text{FID}(4) & \cdots & \text{FID}(N+1) \\ \text{FID}(3) & \text{FID}(4) & \cdots & \cdots & \text{FID}(N+2) \\ \text{FID}(4) & \cdots & \cdots & \cdots & \vdots \\ \vdots & & & & \vdots \\ \text{FID}(N+1) & \text{FID}(N+2) & \cdots & \cdots & \text{FID}(2N) \end{bmatrix}$$

and use $\mathbf{H}_N^{\mathrm{w}} := (\mathbf{L}^{-1})^{\mathrm{T}}\mathbf{H}_N\mathbf{L}^{-1}$ as a finite-dimensional approximation of the canonical correlation operator. Then the singular-value decomposition $\mathbf{H}_N^{\mathrm{w}} = \mathbf{U\Sigma V}$ is formed; i.e., $\mathbf{\Sigma}$ is diagonal with strictly positive diagonal entries $\mathbf{VV}^* = \mathbf{I}$ and $\mathbf{U}^*\mathbf{U} = \mathbf{I}$. Now consider the approximation of $\mathbf{H}_N^{\mathrm{w}}$ given by $\mathbf{\Sigma}_k$, the principal $k \times k$ submatrix of $\mathbf{\Sigma}$; $\mathbf{U}_k$, the matrix made up of the first k columns of $\mathbf{U}$; and $\mathbf{V}_k$, the matrix made up of the first k rows of $\mathbf{V}$; i.e., $\mathbf{H}_N^{\mathrm{w}} = (\mathbf{L}^{-1})^{\mathrm{T}}\mathbf{H}_N\mathbf{L}^{-1} \approx \mathbf{U}_k\mathbf{\Sigma}_k\mathbf{V}_k$. Hence $\mathbf{H}_N \approx \mathbf{L}^{\mathrm{T}}\mathbf{U}_k\mathbf{\Sigma}_k\mathbf{V}_k\mathbf{L}$. Setting $\mathcal{O}_k := \mathbf{L}^{\mathrm{T}}\mathbf{U}_k\mathbf{\Sigma}_k^{1/2}$, $\mathcal{R}_k := \mathbf{\Sigma}_k^{1/2}\mathbf{V}_k\mathbf{L}$, we obtain a full rank factorization of $\mathbf{H}_N$, $\mathbf{H}_N \approx \mathcal{O}_k\mathcal{R}_k$ and the method described earlier to estimate the parameters of the FID from $\mathcal{O}_k$, $\mathcal{R}_k$ can be used with the slight modification that $\mathbf{C}_k$ is such that $\mathbf{C}_k\mathbf{A}_k$ is the first row of $\mathcal{O}_k$. This modification is necessary to deal with the redefinition of the Hankel operator.

It follows from the theory of stochastic realization and approximation (6, 7) that the parameters obtained give rise to a simulated FID whose Fourier transform is positive real, i.e., is properly phased in the infinite-data case. The above-mentioned references are applicable to our situation since the stochastic realization and approximation problem is mathematically equivalent to the problem of analyzing an FID whose discrete Fourier transform has positive real part.

However, in the finite-data case, this is only approximately guaranteed. It should also be pointed out that, in the infinite-data case, the approximation step of going from $\mathbf{U}$, $\mathbf{\Sigma}$, $\mathbf{V}$ to $\mathbf{U}_k$, $\mathbf{\Sigma}_k$, $\mathbf{V}_k$ does not destroy proper phasing if $\mathbf{U}$, $\mathbf{\Sigma}$, $\mathbf{V}$ is a singular-value decomposition of the infinite data matrix. This

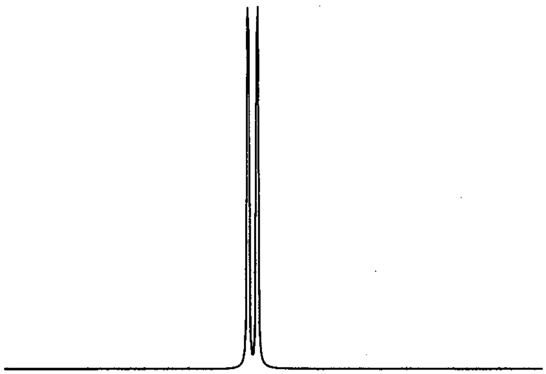

FIG. 2. Spectrum of FID as in Fig. 1 after processing with the modified Hankel-matrix-based method ($k = 2$).

is the essence of the "stochastic balanced-approximation method" (7).

For example, due to noise and other disturbances, F may not be of positive type, even if this were the case in the noise-free situation. But if F is not of positive type the factorization $\mathbf{T}_N = \mathbf{L}^*\mathbf{L}$ may not exist. Then a positive diagonal matrix should be added to $\mathbf{T}_N$ to ensure that the factorization exists. If this alternative method is applied to the simulated FID that was used in Fig. 1a and Fig. 1b, a properly phased Fourier transform is obtained as shown in Fig. 2. The algorithms were implemented in MATLAB Version 4.1.

In summary, it is demonstrated that NMR spectral analysis methods using a singular-value decomposition of the Hankel matrix made up of the elements of the FID can lead to phasing problems. We propose modifying this method by suitably weighting the Hankel matrix. In the infinite-data case this modification is guaranteed to produce a correctly phased Fourier transform. Using an example it is shown that also in the finite-data case the method leads to a well phased spectrum. This method could be of general use in automated data processing since it has the well-known noise-reduction properties of the singular-value-decomposition-based methods and avoids one of its shortcomings.

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