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A new subspace-based method for determining common signal poles in multichannel signals [1]

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Abstract

The goal of the paper is to determine the common dynamics or signal poles in two signals. To perform this task the two signals are stacked in Hankel matrices. By the determination of the intersection of the column spaces of two Hankel matrices, the common signal poles and further on the components having proportionally varying amplitudes are detected. The algorithm was tested by Monte-Carlo simulations on a set of simulation signals.

Key words: multichannel, parameter estimation

0.1 Introduction

A time-domain NMR free induction decay (FID) experiment can be modeled as a sum of complex damped exponentials:

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$$x(n) = \sum_{s=1}^{s=S} A(s) e^{i\tilde{\phi}(s)} e^{(-\alpha(s)+i2\pi\nu(s))t(n)} + \quad (1)$$
$$e(n), n = 0, \ldots, N-1$$

where S is the number of complex damped exponentials, $A \in \mathbb{R}^{S\times 1}$ contains the amplitudes, $\alpha \in \mathbb{R}^{S\times 1}$ contains the damping factors, $\nu \in \mathbb{R}^{S\times 1}$ contains the frequencies (in Hz) and $\tilde{\phi} \in \mathbb{R}^{S\times 1}$, $\tilde{\phi}(s) = \phi(s) + \phi_0, s = 1, \ldots, S$ with $\phi(s), s = 1, \ldots, S$ the phases of the S components and ϕ_0 the zero-order phase. Furthermore, $e(n)$ is complex white Gaussian noise. The number of complex data points is represented by N. The discretely sampled time steps are $t(n) = (n + \eta)\Delta t$, with $t(0) = \eta\Delta t$ the begin time or dead time of the spectrometer and Δt the sampling interval. The phases $\phi(s)$, required only under particular experimental conditions, can usually be set equal to zero as will be assumed in the remainder of the paper. Another way of writing Eq. 1 is the following:

$$x(n) = \sum_{s=1}^{S} c(s) z(s)^{(n+\eta)}, \quad (2)$$
$$n = 0, \ldots, N-1,$$
$$\text{with } c(s) \equiv A(s) e^{i\tilde{\phi}(s)} \text{ and}$$
$$z(s) \equiv e^{(-\alpha(s)+i2\pi\nu(s))\Delta t}$$

where $c(s), s = 1, \ldots, S$ are the so-called complex amplitudes and $z(s), s = 1, \ldots, S$ are the so-called signal poles.
Now we consider 2 FIDs $x_1(n)$ and $x_2(n)$ with

$$x_1(n) = \sum_{s=1}^{s=S_1} A_1(s) e^{i(\tilde{\phi}_1(s))} e^{(-\alpha_1(s)+i2\pi\nu_1(s))t(n)} \quad (3)$$

$$x_2(n) = \sum_{s=1}^{s=S_2} A_2(s) e^{i(\tilde{\phi}_2(s))} e^{(-\alpha_2(s)+i2\pi\nu_2(s))t(n)} \quad (4)$$

where the different quantities are defined in a way similar as in Eq. 1.
What basically happens in the algorithm is a time-domain fit of the FIDs x_1 and x_2 using the proposed model function of complex damped exponentials. A naive implementation would be to determine first the parameters of the model function for FID x_1 and then for FID x_2. The result would be two sets of parameters: $A_1(s), \alpha_1(s), \nu_1(s), \tilde{\phi}_1(s), s = 1, \ldots, S_1$ and $A_2(s), \alpha_2(s), \nu_2(s), \tilde{\phi}_2(s), s = 1, \ldots, S_2$. The next step in the procedure would then be looking for common signal poles, i.e. components for which $-\alpha_1(p) + i2\pi\nu_1(p) \equiv z_1(p) = z_2(q) \equiv -\alpha_2(q) + i2\pi\nu_2(q)$ for some p and q. The reason for looking for common signal poles is obvious: only signal poles representing metabolites that are present in signal $x_1(n)$ (obtained from the control sample) as well as in signal $x_2(n)$ (ob-

tained from the treated sample) can give rise to proportional changes in their corresponding spectral intensities, i.e. amplitudes $A_1(s)$, $A_2(s)$. In a typical experiment a majority of the spectral intensities of the S_c common signal poles scale with a factor R (the latter of course corresponds to the normalization factor that will be computed) whereas the signal poles whose corresponding spectral intensities do not scale with this factor R belong to metabolites whose concentration on the cellular level has been changed by a particular physical, chemical, or biological agent. It is clear that the above described straightforward approach works perfectly for **noiseless** signals x_1 and x_2. However, in real-life experiments signals x_1 and x_2 are contaminated by complex white Gaussian noise e_1 and e_2 and only x_{1n} and x_{2n} are observed:

$$x_{1n}(n) = x_1(n) + e_1(n) \text{ and } x_{2n}(n) = x_2(n) + e_2(n).$$

Furthermore, the involved signal poles can lie very close to each other. In such circumstances it will be extremely difficult –if not impossible– to detect common signal poles, i.e. determine which signal pole of x_{1n} corresponds to which signal pole of x_{2n}. A more advanced technique is called for in the noisy case and will be described in the next paragraph.
To explain the algorithm we start again from the noiseless case. The algorithm starts by stacking x_1 and x_2 in $L \times M$ Hankel matrices H_1 and H_2:

$$H_1 \equiv \begin{bmatrix} x_1(0) & x_1(1) & \dots & x_1(M-1) \\ x_1(1) & x_1(2) & \dots & x_1(M) \\ \vdots & \vdots & \vdots & \vdots \\ x_1(L-1) & x_1(L) & \dots & x_1(N-1) \end{bmatrix} \text{ and}$$

$$H_2 \equiv \begin{bmatrix} x_2(0) & x_2(1) & \dots & x_2(M-1) \\ x_2(1) & x_2(2) & \dots & x_2(M) \\ \vdots & \vdots & \vdots & \vdots \\ x_2(L-1) & x_2(L) & \dots & x_2(N-1) \end{bmatrix},$$

with M chosen greater than S_1 and S_2 and subject to the constraint $N = M + L - 1$. Before we proceed with the explanation of the procedure to find the common signal poles, it is useful to clarify the link that exists between the representation (see Eq. 2) of a signal consisting of a sum of complex damped exponentials, such as x_1, and the Hankel matrix built from that signal, namely H_1. The relationship is expressed by the Vandermonde decomposition of the Hankel matrix:

$$H_1 = O_1 D_1 C_1^T \tag{5}$$

$$\text{with } O_1 \equiv \begin{bmatrix} 1 & 1 & \dots & 1 \\ z_1(1) & z_1(2) & \dots & z_1(S_1) \\ \vdots & \vdots & \vdots & \vdots \\ z_1(1)^{L-1} & z_1(2)^{L-1} & \dots & z_1(S_1)^{L-1} \end{bmatrix},$$

$$D_1 \equiv \begin{bmatrix} c_1(1) & 0 & \dots & 0 \\ 0 & c_1(2) & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & c_1(S_1) \end{bmatrix} \text{ and}$$

$$C_1 \equiv \begin{bmatrix} 1 & 1 & \dots & 1 \\ z_1(1) & z_1(2) & \dots & z_1(S_1) \\ \vdots & \vdots & \vdots & \vdots \\ z_1(1)^{M-1} & z_1(2)^{M-1} & \dots & z_1(S_1)^{M-1} \end{bmatrix}.$$

From the latter equations, it follows that the column space of the matrix H_1 is determined by the vectors $v_{1k} \equiv [1 \ z_1(k) \ z_1(k)^2 \ \dots z_1(k)^{L-1}]^T, k = 1, \dots, S_1$. Therefore if the signals x_1 and x_2 have S_c signal poles in common, the corresponding vectors $v_{1j}, j = 1, \dots, S_c$ form a basis for the intersection of the column spaces of H_1 and H_2 [3]. Therefore, to find the common signal poles first the intersection of the column spaces of H_1 and H_2 is determined and next the signal poles can be extracted from this common subspace. Finding the intersection of the column spaces of H_1 and H_2 can easily be done as follows:

$$H_1 X = H_2 Y$$

$$[H_1 \ H_2] \begin{bmatrix} X \\ -Y \end{bmatrix} = 0,$$

and next use the Singular Value Decomposition (SVD) of $[H_1 \ H_2] = U_{ex} S_{ex} V_{ex}^H$ to find X and Y:

[3] It can easily be proven that no vector other than the signal vectors coming from common signal poles lie in the common subspace. The proof relies entirely on the fact that a matrix like O_1 (see Eq. 5) cannot be rankdeficient if the signal poles are distinct.

$$X = V_{ex}(1 : M, S_1 + S_2 - S_c + 1 : 2M) \qquad (6)$$
$$Y = -V_{ex}(M + 1 : 2M, S_1 + S_2 - S_c + 1 : 2M).$$

Note that the column space of the matrix $H_c \equiv H_1 X = H_2 Y$ is the intersection of the column spaces of H_1 and H_2.
Due to the shift-invariant structure of the matrix H_c it is now straightforward (see next sections) to determine the common signal poles $z_1(k) = z_2(k), k = 1, \ldots, S_c$.
Once the common poles are calculated, the remaining poles in x_1 and x_2 are determined. Note that at this point, the situation corresponds to the case in which we have some a priori known signal poles (in this case these are the now available common signal poles) and we have to determine the remaining poles [2,1]. As shown in [2,1] and briefly summarized in the next sections, the remaining signal poles can easily be determined, by projecting the row spaces of H_1 and H_2 onto the orthogonal complement of the subspace spanned by the common signal poles and their powers. This projection allows the computation of the remaining signal poles $z_1(k), k = S_c + 1, \ldots, S_1$ of x_1 and the remaining signal poles $z_2(k), k = S_c + 1, \ldots, S_2$ of x_2. Using the determined signal poles and the model function Eq. 3, it is straigthforward to find the amplitudes $A_1(k), k = 1, \ldots, S_1$ and phases $\tilde{\phi}_1(k), k = 1, \ldots, S_1$ of x_1, simply by solving the following set of equations:

$$L_1 c_1 = x_1 \qquad (7)$$
$$\text{with } L_1 \equiv \begin{bmatrix} 1 & 1 & \ldots & 1 \\ z_1(1) & z_1(2) & \ldots & z_1(S_1) \\ \vdots & \vdots & \vdots & \vdots \\ z_1(1)^{N-1} & z_1(2)^{N-1} & \ldots & z_1^{N-1} \end{bmatrix}.$$

In a similar way, the amplitudes $A_2(k), k = 1, \ldots, S_2$ and phases $\tilde{\phi}_2(i), k = 1, \ldots, S_2$ of x_2 are found.
Let us now consider what changes when the above described subspace procedure is applied to the observed **noisy** signals x_{1n} and x_{2n} instead of to the noiseless signals x_1 and x_2. Obviously Eq. 5 is no longer satisfied exactly for the simple reason that H_1 no longer has rank S_1. Nevertheless it is still possible to determine an *estimate* of the common subspace and thus an *estimate* of the common signal poles. To be more specific the noisy signals lead to a set of inconsistent equations 13 that will be solved in a Total Least Squares (TLS) sense. As in the noiseless case, the determination of the "uncommon" signal poles leads to a system of Eq. 19. However, in the noisy case the latter system of equations is inconsistent and will be solved in a TLS sense. Finally, system 7 –used for the determination of the complex amplitudes– becomes inconsistent in the noisy case and will be solved in a Least Squares (LS) sense.

As mentioned at the beginning of this section, the spectral intensities (i.e. the amplitudes in A_1 and A_2) of S_p components will present proportional changes due to different cell concentrations while the spectral intensities of $S_c - S_p$ components will present nonproportional changes, which can most likely be attributed to the effects of a particular agent. Therefore, in order to find the correct normalization factor we proceed in the following way. Set $r \equiv A_2(1:S_c,1)./A_1(1:S_c,1)$, where "./" represents the pointwise division of two vectors. Next, signal pole $z_1(1) \equiv z_2(1)$ is assigned to class 1, Next, we check if $r(2)$ lies close to $r(1)$ by evaluating $\|r(2) - r(1)\|/r(1) < 0.1$[4]. If this is true, the signal pole $z_1(2) \equiv z_2(2)$ is assigned to class 1 as well. If $r(2)$ is not close to $r(1)$, a new class, class 2 is created and the second common signal pole $z_1(2) \equiv z_2(2)$ is assigned to the latter class, ... In the end the class with the largest number of signal poles determines the normalization factor, simply by taking the mean of the elements $r(i)$ that correspond to the signal poles of the largest class. The entire procedure can be described in the following schematic way:[Algorithm1(S_1, S_2, S_c)]

1. **begin**
2. $(\alpha_{1,2}(s), \nu_{1,2}(s), s = 1, \ldots, S_c)$:=
   common_sp(x_1, x_2);
   /*compute the common signal poles of x_1 and x_2*/
3. $(\alpha_1(s), \nu_1(s), s = S_c + 1, \ldots, S_1)$:=
   diff_sp$(x_1, S_1, \alpha_1(s), \nu_1(s), s = 1, \ldots, S_c)$
   /*compute the remaining signal poles of x_1*/
4. $(\alpha_2(s), \nu_2(s), s = S_c + 1, \ldots, S_2)$:=
   diff_sp$(x_2, S_2, \alpha_2(s), \nu_2(s), s = 1, \ldots, S_c)$
   /*compute the remaining signal poles of x_2*/
5. $(A_1(s), \tilde{\phi}_1(s), s = 1, \ldots, S_1)$:=
   ca$(x_1, \alpha_1(s), \nu_1(s), s = 1, \ldots, S_1)$
   /*compute the complex amplitudes of x_1*/
6. $(A_2(s), \tilde{\phi}_2(s), s = 1, \ldots, S_2)$:=
   ca$(x_2, \alpha_2(s), \nu_2(s), s = 1, \ldots, S_2)$
   /*compute the complex amplitudes of x_2*/
7. R_{est} :=findfactor$(A_1(s), A_2(s), s = 1, \ldots, S_c)$
   /*determine the normalization factor*/
8. **end**.

1 Determination of common signal poles

Here it is shown how the S_c common signal poles can be extracted from the column space of H_c, i.e. the common column space of H_1 and H_2, when both

[4] Note that 0.1 is a user-defined tolerance.

H_1 and H_2 contain respectively the noiseless signal x_1 (see Eq. 3) and x_2 (see Eq. 4).
If $z(1), z(2), \ldots, z(S_c)$ represent the common signal poles, it follows that

$$R(H_c) = R(O), O \in \mathbb{C}^{L \times S_c}$$
$$\text{with } O = \begin{bmatrix} 1 & 1 & \ldots & 1 \\ z(1) & z(2) & \ldots & z(S_c) \\ \vdots & \vdots & \vdots & \vdots \\ z(1)^{L-1} & z(2)^{L-1} & \ldots & z(S_c)^{L-1} \end{bmatrix} \tag{8}$$

and thus

$$\exists B \in \mathbb{R}^{S_c \times (2M - S_1 - S_2 + S_c)} \text{ such that } H_c = OB. \tag{9}$$

Furthermore let

$$H_c = USV^H \tag{10}$$

be the truncated SVD of H_c, with $U \in \mathbb{C}^{L \times S_c}$, $S \in \mathbb{C}^{S_c \times S_c}$, $V \in \mathbb{C}^{S_c \times (2M - S_1 - S_2 + S_c)}$. It then follows from Eq. 9) and Eq. 10

$$\exists \Xi \in \mathbb{C}^{S_c \times S_c} : U = O\Xi \text{ and } SV^H = \Xi^{-1}B, \tag{11}$$

where Ξ is a non-singular matrix. From Eq. 8 it is clear that the column space of H_c is shift-invariant, i.e.

$$\underline{O}Z = \overline{O}, \tag{12}$$

where $\underline{O}$ is the matrix O with its bottom row deleted, $\overline{O}$ is the matrix O with its top row deleted and Z is a diagonal matrix with $z(1), z(2), \ldots, z(S_c)$ on its diagonal. From Eq. 11 and Eq. 12 it then follows that

$$\underline{U}W = \overline{U}, \tag{13}$$

where $W \equiv \Xi^{-1}Z\Xi \in \mathbb{C}^{S_c \times S_c}$, $\underline{U}$ is the matrix U with its bottom row deleted and $\overline{U}$ is the matrix U with its top row deleted. Since by the definition of W, Z and W are related by a similarity transformation, the eigenvalues of Z and W are equal and thus the common signal poles of the noiseless signals x_1 and x_2 can be determined from the left singular vectors corresponding to the S_c largest singular values of H_c by solving 13 followed by the determination of the eigenvalues of the solution.

2 Determination of uncommon signal poles

Here it is shown how –after having determined the common signal poles of the noiseless signals x_1 and x_2– the "uncommon" (i.e. the signal poles contained in x_1 that are different from the common signal poles) signal poles of x_1 (and in a similar way those of x_2) can be determined.
Assume that the signal poles of x_1 are ordered in such a way that $z(i), i = 1, \ldots, S_c$ are the S_c common signal poles. Eq. 5 can be written as follows:

$$H_1 = [O_1' \; O_1''] \begin{bmatrix} D_1' & 0 \\ 0 & D_1'' \end{bmatrix} [C_1' \; C_1'']^T = O_1' D_1' C_1'^T + O_1'' D_1'' C_1''^T, \tag{14}$$

where $O_1' \in \mathbb{C}^{L \times S_c}$, $O_1'' \in \mathbb{C}^{L \times (S_1 - S_c)}$, $D_1' \in \mathbb{C}^{S_c \times S_c}$, $D_1'' \in \mathbb{C}^{(S_1 - S_c) \times (S_1 - S_c)}$, $C_1' \in \mathbb{C}^{M \times S_c}$, $C_1'' \in \mathbb{C}^{M \times (S_1 - S_c)}$. Let the QR factorization of C_1' be represented as follows:

$$C_1' = [Q_1 \; Q_2][R^T \; 0]^T,$$

with $Q_1 \in \mathbb{C}^{M \times S_c}$, $Q_2 \in \mathbb{C}^{M \times (M - S_c)}$, $R \in \mathbb{C}^{S_c \times S_c}$. Therefore it follows that

$$C_1'^T Q_2^* = R^T Q_1^T Q_2^* = R^T (Q_1^H Q_2)^* = 0,$$

where $()^*$ stands for complex conjugate. It is thus clear that

$$H_1 Q_2^* = O_1'' D_1'' C_1''^T Q_2^*. \tag{15}$$

From Eq. 15 it is clear that the column space of $H_1 Q_2^*$ is shift-invariant meaning that

$$\underline{O_1''} Z'' = \overline{O_1''}, \tag{16}$$

where $\underline{O_1''}$ is the matrix O_1'' with its bottom row deleted, $\overline{O_1''}$ is the matrix O_1'' with its top row deleted and Z'' is a diagonal matrix with $z_1(i), i = S_c + 1, \ldots, S_1$, i.e. the uncommon signal poles, on its diagonal. Let

$$H_1 Q_2^* = U S V^H \tag{17}$$

be the truncated SVD of $H_1 Q_2^*$, with $U \in \mathbb{C}^{L \times (S_1 - S_c)}$, $S \in \mathbb{R}^{(S_1 - S_c) \times (S_1 - S_c)}$ and $V \in \mathbb{C}^{(M - S_c) \times (S_1 - S_c)}$. From Eq. 15 and Eq. 17 it follows that

$$\exists \Xi : U = O_1'' \Xi \text{ and } S V^H = \Xi^{-1} D_1'' C_1''^T Q_2^* \tag{18}$$

with $\Xi \in \mathbb{C}^{(S_1-S_c)\times(S_1-S_c)}$ a regular matrix. Combining Eq. 16 and Eq. 18 yields:

$$\underline{U}W'' = \overline{U}, \tag{19}$$

where $W'' \equiv \Xi^{-1}Z''\Xi \in \mathbb{C}^{(S_1-S_c)\times(S_1-S_c)}$, $\underline{U}$ is the matrix U with its bottom row deleted and $\overline{U}$ is the matrix U with its top row deleted. Since by the definition of W'', Z'' and W'' are related by a similarity transformation, the eigenvalues of Z'' and W'' are equal and thus the uncommon signal poles of the noiseless signals x_1 can be determined from the left singular vectors corresponding to the $S_1 - S_c$ largest singular values of $H_1Q_2^*$ by solving Eq. 19 followed by the determination of the eigenvalues of the solution.

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