Improving Parameter Estimation for Surface-NMR Data by Singular Spectrum Analysis Framework

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SUMMARY

A major drawback of applying surface-NMR to hydro-geophysical investigations is high vulnerability to electromagnetic interferences that severely affect the signal quality of surface-NMR measurements. In this paper, we describe an application of a powerful de-noising method based on singular spectrum analysis (SSA) technique. The aim of SSA is to decompose the original time series into a sum of small numbers of independent and interpretable components such as slowly varying trend, oscillatory components, and noise components. The time series is decomposed into noise free original time series components and noise components at the first stage, at the second stage the de-noised time series is reconstructed by using the noise free components extracted from the initial section. The signal retrieval process through the SSA algorithm strongly depends upon two parameters: the window length of the embedding operation and number of needed singular values. To evaluate the performance of the proposed strategy, the method is tested on synthetic signals added to noise-only recordings obtained from surface-NMR field survey. Our results show that the proposed algorithm can enhance the signal to noise ratio significantly, and gives an improvement in estimation of the surface-NMR signal parameters.

Key words: Singular Spectrum analysis; Surface Nuclear Magnetic Resonance; Noise Reduction; Parameter Estimation.

INTRODUCTION

The surface-NMR procedure is a way to quantitatively determine water presence in the subsurface, which is impossible with other geophysical methods available today (Hertrich, 2005). In regard to surface-NMR measurements, environmental and cultural noise is a serious obstacle to achieve reliable results, and limits the widespread use of surface-NMR instruments in hydro-geophysical investigations (Walsh, 2008). Beside the background noise, i.e. random and Gaussian distributed white noise, surface-NMR usually contaminated by different noise sources including power line harmonics and electrical discharges from both natural and artificial sources bringing about spiky events (Dalgaard et al., 2012; Muller-Petke and Costabel, 2014). Technically, in the surface-NMR measurements, typical signal amplitudes are very weak and cannot be easily increased relative to the ambient noise level, hence, it would be quite difficult to reach a reliable result. Consequently, robust and effective noise mitigation approaches are required to acquire the weak surface-NMR signals. Recently, multi-channel surface-NMR systems offer the possibility to measure the time series as broad-band data records at 50 kHz sampling rate instead of providing merely envelopes of the records. Such broad band measurements allow us to implement advanced post-processing techniques for noise reduction. Case histories on suppressing the influence of noise during acquisition and data processing can be found in literature (Trushkin et al. 1994; Legchenko and Valla, 2002; Plata and Rubio, 2002; Walsh, 2008; Strehl, 2006; Dalgaard et al., 2012; Larsen et al., 2013; Muller-Petke and Costabel, 2014; Ghanati et al., 2014; Dalgaard et al., 2014). All approaches have demonstrated useful functionality to further enhancement of the signal to noise ration in surface-NMR measurements. But retrieval of the surface-NMR signal, due to high vulnerability to noise, complex, non-stationary and non-linear nature of it, is still a challenging task. The general objective of this study is to address the application of singular spectrum analysis (SSA) to mitigate harmonic and stochastic (i.e. uncorrelated Gaussian distributed noise and spiky events) noises from surface-NMR signal. After noise removal, signal extraction is performed using the digital quadrature detection with additional phase correction (Muller-petke et al., 2011; Neyer, 2010). The digital quadrature detection turned out to be less sensitive to noise than other methods (e.g. Hilbert transformation, cross-correlation filter, quadrature detection without phase correction) (Neyer, 2010). Subsequently, we consider a regularized Levenberg–Marquardt method for estimating the underlying surface-NMR signal parameters such as initial amplitude V_0, decay time T_2^*, frequency f_0, and phase φ. Whereas an adequate stacking rate of the single records can decrease the power-line interferences due to randomly variation of the phases of the harmonics, so that the intensity at the harmonic frequencies is reduced during the stacking process, the SSA based de-noising is applied on the noise added synthetic Surface-NMR signals after the stacking. The numerical experiments we present show that the proposed method can enhance the signal to noise ratio with an accompanying enhancement in recovery of the signal parameters.

METHOD AND RESULTS

Singular spectrum analysis algorithm

The basic principles of SSA were first emerged in Pike et al. (1984). But what makes its wide applicability is the non-parametric and model-free nature that enables practitioners to deploy it without a prior knowledge of any underlying structure (Chu et al., 2014). The algorithm of SSA consists of two complementary stages: decomposition and reconstruction and both the stages include two distinct steps. In the first stage the observed signal (often called time series) is decomposed and in the second stage the original source signal is reconstructed and used for further analysis. A brief description of the SSA scheme is presented in the following four systematic steps.

Let $S = (s_1, \dots, s_N)$ of length N denote an observed finite realization of a stochastic process. We assume that S has been corrupted by noise.

First stage: Decomposition

1st step: Embedding: To implement the embedding operation we map the one-dimensional time series or signal S into a sequence of lagged vectors of size $\mathcal{W}$ by forming $\mathcal{P} = N - \mathcal{W} + 1$. Define $\mathcal{P}$-lagged vectors $h_1, \dots, h_\mathcal{P}$ by $h_i = [s_i, \dots, s_{i+\mathcal{W}-1}]$, $i = 1, \dots, \mathcal{P}$ and the associated trajectory matrix of the signal S by

$$H = [h_1, h_2, \dots, h_{N-\mathcal{W}+1}] = \begin{bmatrix} s_1 & s_2 & \dots & s_\mathcal{P} \\ s_2 & s_3 & \dots & s_{\mathcal{P}+1} \\ \vdots & \vdots & \ddots & \vdots \\ s_\mathcal{W} & s_{\mathcal{W}+1} & \dots & s_N \end{bmatrix} \quad (1)$$

This process of embedding h into H, fundamental in time series analysis, creates a handle for manipulating rank reduction (Chu et al., 2014).

2nd step: Singular value decomposition (SVD): in the SVD step, we calculate the SVD of the trajectory matrix and represent it as a sum of rank-one bi-orthogonal elementary matrixes. The covariance matrix is calculated, $C = HH^T$, and its decomposition into m eigenvalues $\vartheta_1, \dots, \vartheta_m$ descending order of magnitude $(\vartheta_1 \geq \dots \geq \vartheta_m \geq 0)$ and the corresponding orthogonal eigenvectors $U = (u_1, u_2, \dots, u_m)$ is obtained. Set $J = \max\{i; \text{such that } \vartheta_i > 0\} = rank(H)$ (or $J = min\{\mathcal{W}, \mathcal{P}\}$) and $V_i = H^T \frac{u_i}{\vartheta_i^{(\frac{1}{2})}}$, $i = 1, \dots, J$. The SVD of the Hankel marix H can be written as follows:

$$H = \sum_{i=1}^{J} H_i = \sum_{i=1}^{J} \sqrt{\vartheta_i} u_i V_i^T \quad (2)$$

Where the matrices H_i have rank 1; such matrices are sometimes called elementary matrices. The collection $(\sqrt{\vartheta_i} u_i V_i^T)$ will be called i-th eigentriple of the matrix H, $\sqrt{\vartheta_i}$ $(i = 1, \dots, J)$ are the singular values of the matrix H. It should be noted that the eigenvectors of H arise from the autocorrelation matrix HH^T, the components that present the most coherency in the data will be weighted by singular values with higher values. This way, the decomposition of the trajectory matrix in its singular spectrum is very useful to identify trends in the data. Also, given that the signal in the time series is correlated between time-lagged windows, it will be represented by the largest singular values. Thus, singular values with less weight can be considered as noise components, making possible the use of this tool in noise suppression of time series (Oropeza and Sacchi, 2011).

Second stage: Reconstruction

1st step: Grouping: after obtaining the elementary matrixes in the previous stage, the grouping operation divides the set of indices $\{1, 2, \dots, J\}$ into n disjoint subsets $I_1, \dots, I_n$. Let $I = \{i_1, \dots, i_d\}$, for $d < \mathcal{W}$, be a group of indices $i_1, \dots, i_d$. Then, the matrix H_I corresponding to the group I is defined as $H_I = H_{i1} + \dots + H_{id}$. These matrixes are calculated for $I = I_1, \dots, I_n$ and the expansion (1) leads to the decomposition

$$H = H_{I1} + \dots + H_{In} \quad (3)$$

The process of choosing the set is called the Eigen-triple grouping.

2st step: Diagonal averaging: The purpose of diagonal averaging or Hankelization is to transform a matrix to the form of a Hankel matrix, which can be subsequently converted to a time series length N. For a typical $\mathcal{W} \times \mathcal{P}$ matrix H with elements h_{ij}, $1 \leq i \leq \mathcal{W}$, $1 \leq j \leq \mathcal{P}$, we set $\mathcal{W}^* = \min(\mathcal{W}, \mathcal{P})$, $\mathcal{P}^* = \max(\mathcal{W}, \mathcal{P})$ and $N = \mathcal{P} + \mathcal{W} - 1$. By making the diagonal averaging we transfer the matrix H into the series $g_1, \dots, g_N$ through the following formula:

$$g_k = \begin{cases} \frac{1}{k} \sum_{m=1}^{k} g(m, k-m+1) & For\ 1 \leq k \leq \mathcal{W}^* - 1 \\ \frac{1}{\mathcal{W}^*} \sum_{m=1}^{\mathcal{W}^*} g(m, k-m+1) & For\ \mathcal{W}^* \leq k \leq \mathcal{P}^* \\ \frac{1}{N-k+1} \sum_{m=k-\mathcal{P}^*+1}^{\mathcal{W}^*} g(m, k-m+1) & For\ \mathcal{P}^* + 1 \leq k \leq N \end{cases} \quad (4)$$

The whole procedure of the SSA scheme strongly depends upon two basic parameters that must be assigned or chosen by the practitioner, namely, (i) the window length of the embedding and (ii) the number of singular values (a modeling parameter). Certainly, the values chosen for $\mathcal{W}$ and $\mathcal{R}$ will interact one with another so as to effect performance and it is vital to ensure that the techniques employed for assignment and choice of the two parameters yield appropriate separability between signal and noise components as well as minimize reconstruction error. Standard practice in SSA is to use a value for the window length large enough to ensure that the signal and noise components are strongly separated. Several attempts have been made in the mathematical context to select the appropriate values of parameters $\mathcal{W}$ and $\mathcal{R}$. To obtain the optimal values of $\mathcal{W}$ and $\mathcal{R}$, we consider the separability between signal and noise components which is an indispensable concept in studying SSA properties. The degree of approximate separability between two signals $\mathbb{S}^{(1)}$ and $\mathbb{S}^{(2)}$ is quantified by the so-called weighted-correlation (or W-correlation) criterion which is defined as follows:

$$\rho_{1,2}^{W} = \frac{\sum_{j=1}^{N} W_j^{\mathcal{W},N} \mathbb{S}_j^{(1)} \mathbb{S}_j^{(2)}}{\sqrt{\sum_{j=1}^{N} W_j^{\mathcal{W},N} (\mathbb{S}_j^{(1)})^2 \times \sum_{j=1}^{N} W_j^{\mathcal{W},N} (\mathbb{S}_j^{(2)})^2}} \quad (5)$$

Where $W_j^{\mathcal{W},N} = \min\{j, N-j+1\}$ and $2 < \mathcal{W} < N-1$.

If the absolute value of the W-correlations is small, then the corresponding signals are almost W-orthogonal, but, if it is large, then the two signals are far from being W-orthogonal and are therefore weakly separable. In other words, the value of the W-correlations indicates that how the reconstructed signal has been separated from the noise component.

Numerical results

In this section, to demonstrate the functionality of the proposed algorithms, numerical experiments from the modeling of a synthetic signal added to real noise recordings are tested. The quality of the reconstructions is measured in terms of the signal to noise ratio (SNR) in decibels (dB). In addition, the mean absolute percentage error (MAPE) is quoted in this paper for evaluating estimation accuracy. In brief, the lower the MAPE value, the better the performance.

$$\text{MAPE} = \frac{1}{N} \sum_{i=1}^{N} \left| 100 \times \frac{(s(t_i) - \hat{s}(t_i))}{s(t_i)} \right|, \quad (6)$$

Where $\hat{s}(t_i)$ is the reconstructed signal (the processed and stacked signal) and $s(t_i)$ is the original signal. 35 recorded noises received by the Numis-Poly system are used to be fully ensured of the noise simulation instead of producing artificial noises. The synthetic surface-NMR signal with $V_0 = 200$ nV, $T_2^* = 250$ ms, $F_0 = 2138$ Hz and $\phi = 1.03$ rad is simulated through Eq. (7), and then the noise-only recodes are added to it.

$$V(t) = V_0 \exp(-t/T_2^*) \cos(2\pi F_0 t + \phi) \quad (7)$$

In Eq. (7), the initial amplitude and decay time of the FID signal is denoted by V_0 and T_2^*, the phase of the retrieved signal enters as ϕ, F_0 indicates the Larmor frequency.

It is well-known that by increasing the stack size further reduction of the coherence noise is provided. This is caused by the fact, that the phases of the power-line harmonics randomly changed in every single stack, so that the energy at the harmonic frequencies is diminished during the stacking process (Strehl, 2006). Hence, the proposed de-noising algorithm is implemented on the stacked signal. the corresponding surface-NMR signal is generated using the stacking of the synthetic MRS signal superimposed on real MRS noise records, as shown in Figure 1 (grey). Knowing the significance of the appropriate choice of $\mathcal{W}$ and $\mathcal{R}$ from the previous section, we use the W-correlation criterion to obtain the optimal values of the two parameters, leading eventually to better reconstruction of the surface-NMR signal. According to the results derived from the W-correlation criterion (not shown here), we can conclude that choosing window length equal to 5223 and $\mathcal{R}$ equal to 2 gives best separation between signal and noise components. On the other hand, the W-correlation value in terms of a fixed value of $\mathcal{R}$ for large and small values of $\mathcal{W}$ is far away from the minimum W-correlation. Here, we use as signal the reconstructed series containing optimal $\mathcal{R}$ components and select the remaining $\mathcal{R}$, which does not belong to the reconstruction, as noise. The result of SSA-based filtering with the optimum values of parameters $\mathcal{W}$ and $\mathcal{R}$ is presented in Figure 1 (black).). In this Figure it is possible to observe the characteristics of a MRS signal. Figure 2 displays the power spectrum corresponding to a single, unfiltered noise-only record with synthetic signal added (black), unfiltered and stacked signal (blue) as well as filtered and stacked signal (grey). It can be seen that the power-line harmonics have been considerably removed through the proposed SSA based de-noising algorithm. The peak at the Larmor frequency is left undisturbed. In addition, the signal-to-noise ratio increases from 0.36 dB (related to the noisy FID signal) to 19.7 dB. When comparing the spectrum of the single, unprocessed record and the corresponding spectrum of the stacked and unprocessed signal, we note that the stacking operation has led to a partly reduction of the power-line harmonics. After the application of the SSA based filtering, the next step is the envelope detection and fitting the envelope to the mono-exponential decay. Here, the digital quadrature detection with phase correction is used to extract the MRS signal envelope. Subsequently, in order to estimate the signal parameters, a non-linear optimization problem based on the regularized Levenberg–Marquardt method (Chavent, 2009) must be used. The fitting yields the relaxation time T_2^* and the initial value after the end of the excitation signal. Representative results from the proposed method to retrieve the MRS signal parameters are reported in Table 1. For comparison the MRS signal has been also recovered in the case where no processing has been carried out. One can see that the value of MAPE obtained by using the proposed algorithm is lower than that of merely use of pure stacking (plain averaging over the signal records). Moreover, in Figures 3(a)-(b), the signal envelope (dark line) and exponential decay curve (red line) defined by the fit-parameters V_0 and T_2^* to the signal envelope associated to the unfiltered and filtered signal are illustrated.

CONCLUSIONS

In this paper, we suggested an efficient post-processing workflow based on the singular spectrum analysis for attenuating stochastic and harmonic noises from surface-NMR measurements which leads to an increase in the accuracy of the parameter estimation. The SSA algorithm contains two stages referred to as Decomposition and Reconstruction, whilst the two choices are known as the window length $\mathcal{W}$ and the number of singular values $\mathcal{R}$. Each of the two stages includes two separate steps known as Embedding operation, Singular Value Decomposition (SVD) and, grouping and Diagonal averaging. We considered the concept of separability between the signal and noise components through measure of weighted-correlation criterion to determine the optimal value of parameters $\mathcal{W}$ and $\mathcal{R}$. The digital quadrature detection with phase correction was used to extract the envelope of the FID signal. Subsequently, we applied a non-linear optimization problem based on the regularized Levenberg–Marquardt method to the mono-exponential decay curve to estimate the signal parameters. The results of numerical experiments from applying the proposed filtering approach to the real noise-only measurements and synthetic signal added to noise-only records confirmed relatively high performance of the proposed scheme in suppression of electromagnetic interferences that allows more accurate retrieval of the model parameters.

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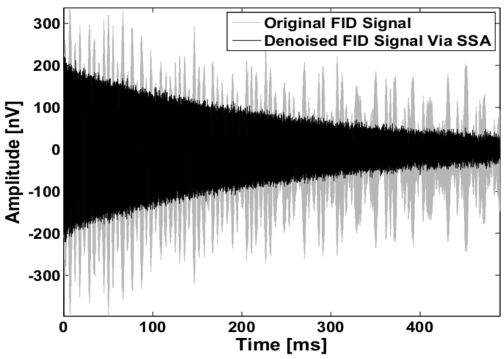

Figure 1. The unprocessed synthetic MRS curve (stack of 32 records) is grey and the processed signal using the SSA algorithm is black.

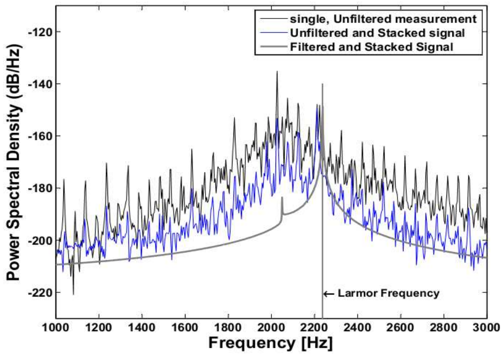

Figure 2. Representation of the power spectral density corresponding to a single, unfilterled noise-only record with synthetic signal added (black), unfilterd and stacked signal (blue) and filterd and stacked signal (grey). The Larmor frequency is indicated in the figure by grey line.

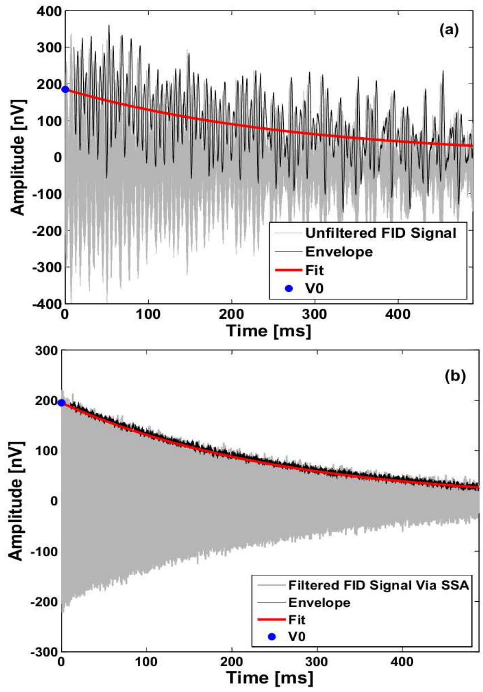

Figure 3. FID curves before (a) and after (b) the application of the SSA-based de-noising algorithm. Oscillating gray line, simulated time series; black line, signal envelope; red line, exponential decay curve defined by the fit-parameters V_0 and T_2^*; dot, initial amplitude of the estimated signal.

Model Parameters	Estimated Parameters via Pure Staking	Estimated Parameters via SSA-Based Filtering
V_0	187.1	197.82
T_2^*	288.8	258.9
f_0	2237.02	2237.9
φ	0.92	0.993
MAPE[a] [%]	8.89	0.71

[a] **MAPE: Mean Absolute Percentage Error**

Table 1. Estimated value of the four parameters using pure stacking and SSA-based filtering method on a synthetic MRS signal corrupted by noise-only recordings.