An ESPRIT-based parameter estimator for spectroscopic data

Gudmundson, Erik; Wirfält, Petter; Jakobsson, Andreas; Jansson, Magnus

Published in:
2012 IEEE Statistical Signal Processing Workshop (SSP), Proceedings of

DOI:
10.1109/SSP.2012.6319820

2012

Link to publication

Citation for published version (APA):

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
• You may not further distribute the material or use it for any profit-making activity or commercial gain
• You may freely distribute the URL identifying the publication in the public portal

Take down policy
If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.
An ESPRIT-based parameter estimator for spectroscopic data

E. GUDMUNDSON, P. WIRFÄLT, A. JAKOBSSON, AND M. JANSSON

Published in: Proceedings of the IEEE Statistical Signal Processing Workshop (SSP’12), August 5-8, 2012, Ann Arbor, MI, USA
AN ESPRIT-BASED PARAMETER ESTIMATOR FOR SPECTROSCOPIC DATA

Erik Gudmundson*, Petter Wirfält*, Andreas Jakobsson†, and Magnus Jansson*

*ACCESS Linnaeus Center, Signal Processing, KTH Royal Institute of Technology, Sweden
†Dept. of Mathematical Statistics, Lund University, Lund, Sweden

ABSTRACT

The pulse spin-locking sequence is a common excitation sequence for magnetic resonance and nuclear quadrupole resonance signals, with the resulting measurement data being well modeled as a train of exponentially damped sinusoids. In this paper, we derive an ESPRIT-based estimator for such signals, together with the corresponding Cramér-Rao lower bound. The proposed estimator is computationally efficient and only requires prior knowledge of the number of spectral lines, which is in general available in the considered applications. Numerical simulations indicate that the proposed method is close to statistically efficient, and that it offers an attractive approach for initialization of existing statistically efficient gradient search based techniques.

Index Terms— Parameter estimation; damped sinusoids; subspace techniques; multidimensional signal processing; NQR; NMR

1. INTRODUCTION AND DATA MODEL

Spectral estimation is a classical problem which has found applications in a wide variety of fields, such as astronomy, medical imaging, radar, and spectroscopic techniques (for example magnetic resonance, NMR, and nuclear quadrupole resonance, NQR). Subspaced-based estimators form an important class of spectral estimation methods that have proven to be useful for estimation of both damped and undamped sinusoidal signals (see, e.g., [1, 2]). Even though much work has been done on the estimation of damped and undamped sinusoids, there are only a few algorithms dealing with structured data models able to fit data produced by magnetic and quadrupolar resonance techniques. Such measurements are often resulting from the use of pulse spin-locking (PSL) sequences, which will then induce a fine structure into the signals. The PSL sequence consists of a preparatory pulse and a train of refocusing pulses, where the time between two consecutive refocusing pulses is 2τ, as illustrated in Fig. 1. As discussed in [3, 4], the signal resulting from a PSL excitation can be well modeled as

\[ y_{m,t} = x_{m,t} + w_{m,t}, \quad (1) \]

where \( m = 0, \ldots, M - 1 \) denotes the echo number, and \( t = t_0, \ldots, t_{N-1} \) the local time within each echo, with \( t = 0 \) denoting the center of the current pulse, and where we assume uniform sampling intervals within each echo. Moreover, \( w_{m,t} \) is an additive circular symmetric white Gaussian i.i.d. noise with variance \( \sigma^2 \), and

\[ x_{m,t} = \sum_{k=1}^{K} \alpha_k \exp \left( \imath \omega_k t - \beta_k |t - \tau| - (t + 2\tau m) \eta_k \right), \quad (2) \]

with

\[ \alpha_k \triangleq \begin{cases} \alpha_k \exp(-\beta_k \tau) \cdot \exp(-2\eta_k \tau m) & \text{for } t < \tau, \\ \alpha_k \exp(\beta_k \tau) \cdot \exp(-2\eta_k \tau m) & \text{for } t \geq \tau, \end{cases} \]

\[ \beta_k \triangleq \begin{cases} \exp(i\omega_k) \cdot \exp(\beta_k - \eta_k) & \text{for } t < \tau, \\ \exp(i\omega_k) \cdot \exp(-\beta_k - \eta_k) & \text{for } t \geq \tau, \end{cases} \]

This work was supported in part by the Swedish Research Council, Carl Trygger’s foundation, and the European Research Council (ERC, grant agreement numbers 228044 and 261670).
the same subspace. Regrettably, only $t < \tau$ may partition each echo into two parts, based on (4) and (5), such as either one or two-sided signals. For scenarios when measurement (SVD) of $S_{\eta}(k, \tau) = 1$.

$$X_m = \begin{bmatrix} x_{m,t_0} & x_{m,t_1} & \cdots & x_{m,t_{L-1}} \\ x_{m,t_1} & x_{m,t_2} & \cdots & x_{m,t_L} \\ \vdots & \vdots & & \vdots \\ x_{m,t_{L-1}} & \cdots & \cdots & x_{m,t_N} \end{bmatrix} \in \mathbb{C}^{L \times L'}$$

where $L' = N - L + 1$. This (noise-free) echo matrix may then be collected, and partitioned, as

$$X = [X_0 \cdots X_{M-1}] = S \begin{bmatrix} C_m & T^T \end{bmatrix}$$

where $S \in \mathbb{C}^{L \times K}$, $[S]_{l,k} = z_{l-1}^{(l)}$, $T \in \mathbb{C}^{L \times K}$, $[T]_{m,k} = z_{m}^{(m)}$.

Thus, $S$ and $T$ may be factored from each $X_m$, as in (7) due to $z_k$ in (5) being independent of $m$. Forming the singular value decomposition (SVD) of $X$, i.e.,

$$X = U \Sigma V^H,$$

it may be noted by comparing (7) and (8) that $S$ and $U$ will span the same subspace. Regrettably, only $y_{m,t}$, i.e., the noise-corrupted measurements of (2) are available, instead necessitating the forming of $y_m$ and $Y$ from $y_{m,t}$ similarly to (6) and (7).

Typically, magnetic resonance measurements may be obtained as either one or two-sided signals. For scenarios when measurements of both the expanding and the decaying part of the signal are available, so-called two-sided echoes, as is illustrated in Fig. 1, one may partition each echo into two parts, based on (4) and (5), such that one part is formed from $t < \tau$ and the other from $t \geq \tau$. Thus,

$$y_m = \begin{bmatrix} y_{m,t_0} & \cdots & y_{m,t_{N-1}} \end{bmatrix}^T \triangleq \begin{bmatrix} y_m^{(+)T} \\ y_m^{(-)T} \end{bmatrix},$$

where the superscripts $y_m^{(+)}$ and $y_m^{(-)}$ have been introduced to denote the expanding ($t < \tau$) and decaying ($t \geq \tau$) parts of $y_m$, respectively. One then forms $Y^{(+)}$ using only $y_m^{(+)}$, and similarly for $Y^{(-)}$. The following estimation is then performed independently for each of $Y^{(+)}$ and $Y^{(-)}$; accordingly, one gets two independent estimates for each parameter, i.e., $\hat{c}_k^{(+)}$ and $\hat{c}_k^{(-)}$. These are then combined to form the estimate $\hat{c}_k = \frac{1}{2} \hat{c}_k^{(+)} + \frac{1}{2} \hat{c}_k^{(-)}$, where $\hat{c}_k$ represents $\hat{c}_k$, $\eta_k$, $\omega_k$, as appropriate.

Alternatively, for cases when only one-sided echoes are available, i.e., when one only obtains measurements for the decaying part $y_m^{(-)}$, for $t \geq \tau$, the analysis is analogous, although with appropriate changes dictated by (4)-(6). In order to simplify the notation, we omit the superscript $(-)$ in the following.

Proceeding with either forms of measurements, let $X^\dagger$ denote the operation of removing the bottom-most row of the matrix $X$, and similarly let $X^\ddagger$ denote removal of the top-most row. Then, it is easily seen that $S^\dagger = S^\ddagger Z$, where

$$Z = \text{diag}\{z_1, \ldots, z_K\},$$

and hence $U^\dagger = U^\ddagger \Omega$, where $\Omega$ and $Z$ are related by a similarity transformation and thus have the same eigenvalues. Using the measured data, the SVD of $Y$ is formed, yielding

$$Y = U \Sigma \hat{V}^H + W,$$

where $\Sigma$ denotes the matrix formed from the $K$ largest singular values and $U$ and $\hat{V}$ denote the matrices formed by the corresponding singular vectors. The residual term, $W$, contains the noise. The total-least squares (TLS) estimate $\hat{\Omega}$ of $\Omega$ may then be formed from $\hat{U}^\dagger = \hat{U}^\ddagger \hat{\Omega}$,

and we may obtain estimates of the $K$ poles $\{\hat{z}_k\}_{k=1}^K$ from the eigenvalues of $\hat{\Omega}$. Using (5), we then find $\hat{\omega}_k = \angle \hat{z}_k$ and $\hat{\beta}_k + \hat{\eta}_k = -\log |\hat{z}_k|$. With the estimated poles, one may then, for each echo $m$, write

$$\begin{bmatrix} z_{m,0}^{(+)T} \\ \vdots \\ z_{m,N-1}^{(+)T} \end{bmatrix} \hat{c}_m \begin{bmatrix} c_{m,1} \\ \vdots \\ c_{m,K} \end{bmatrix} = \begin{bmatrix} y_{m,0}^{(+)T} \\ \vdots \\ y_{m,N-1}^{(+)T} \end{bmatrix}$$

which forms a regular LS problem for $\{\hat{c}_m\}_{k=1}^K$. Using (4), we simplify the notation by introducing $d_k = c_k \alpha_k \exp(\beta_k \tau)$ and then, for each spectral line $k = 1, \ldots, K$, one may form the following LS problem for the estimation of $\{\eta_k\}_{k=1}^K$,

$$\begin{bmatrix} \log |\hat{c}_k| \\ \vdots \\ \log |\hat{c}_{M-1,k}| \end{bmatrix} = \begin{bmatrix} 1 & -2\tau & \cdots \\ \vdots & \vdots & \ddots \\ 1 & -2\tau & (M-1) \end{bmatrix} \begin{bmatrix} \log |d_k| \\ \vdots \\ \eta_k \end{bmatrix},$$

where $\{\hat{c}_m\}_{m=0}^{M-1}$ denote the LS solution to (13). The LS solution to (14) is readily found as

$$\hat{\eta}_k = \frac{3}{M(M-1)-2(M-1)m \log |\hat{c}_m| \log |c_m|^2}. \frac{\tau M(M-1)(M+1)}{\tau M(M-1)(M+1) \log |\hat{c}_m|^2} \log |d_k|,$$

Using (5) and (15), one may then also estimate $\hat{\beta}_k$ as

$$\hat{\beta}_k = -\left(\hat{\eta}_k + \log |\hat{z}_k|\right).$$

Finally, given the estimates $\{\hat{\beta}_k, \hat{\omega}_k, \hat{\eta}_k\}_{k=1}^K$, an estimate of $\alpha_k$, $k = 1, \ldots, K$, may be formed from (1) using a maximum likelihood algorithm, which in this case coincides with the LS solution. Due to space limitations, the reader is referred to, e.g., [3, 6]) for the details.

3. DERIVATION OF THE CRAMÉR-RAO BOUND

We proceed to form the Cramér-Rao Bound (CRB) for the problem at hand, stacking the data from each measurement echo as

$$y = x + w,$$

where $x$ is the parameter vector to be estimated and $w$ is the noise vector. The CRB is given by

$$\text{Var}(x) \geq \frac{1}{\text{Cov}(y, y)},$$

where $\text{Cov}(y, y)$ is the covariance matrix of the data $y$. For the case of a linear model, such as in (17), the CRB can be derived by finding the Fisher information matrix $I(x)$ and taking the reciprocal of its diagonal elements.

$$I(x) = \mathbb{E} \left[ \frac{\partial y}{\partial x} \frac{\partial y}{\partial x}^T \right],$$

where $\mathbb{E}$ denotes the expectation operator. The CRB is then given by

$$\text{Var}(x) \geq \frac{1}{\mathbb{E} \left[ \frac{\partial y}{\partial x} \frac{\partial y}{\partial x}^T \right]}.$$
where
\[
{x} = \begin{bmatrix} x_1^{T} & \cdots & x_{M-1}^{T} \end{bmatrix}^{T} \in \mathbb{C}^{NM \times 1},
\]
\[
x_m = \begin{bmatrix} x_{m,t_0} & \cdots & x_{m,t_{N-1}} \end{bmatrix}^{T} \in \mathbb{C}^{N \times 1},
\]
\[
w = \begin{bmatrix} w_{0,t_0} & \cdots & w_{M-1,t_{N-1}} \end{bmatrix}^{T} \in \mathbb{C}^{N \times 1}.
\]

In order to simplify the notation, let
\[
\xi_k^{m,t} \triangleq \exp(i\omega_k t - \beta_k [t - \tau] - (t + 2\tau m)\eta_k),
\]
so that
\[
x_{m,t} = \sum_{k=1}^{K} \alpha_k \xi_k^{m,t}.
\]
The CRB is given as CRB(\(\gamma\)) = \([\text{FIM}(\gamma)]^{-1}\), where FIM(\(\gamma\)) denotes the Fisher information matrix given the unknown (vector) parameters \(\gamma\), with
\[
\gamma = [a_1, \cdots, a_K, b_1, \cdots, b_K, \omega_1, \cdots, \omega_K, \\
\beta_1, \cdots, \beta_K, \eta_1, \cdots, \eta_K]^{T},
\]
where \(a_k = [\alpha_k]\) and \(b_k = \omega_k\). The CRB for a particular unknown \(\gamma_i\) is then obtained as the \((i, i)\)-th element of the CRB matrix, i.e., CRB(\(\gamma_i\)) = \([\text{CRB}]_{ii}\). From the Slepian-Bang’s formula [1], it is known that
\[
\text{FIM}(\gamma) = \frac{2}{\sigma^2} \text{Re} \left\{ \left( \frac{\partial \gamma}{\partial \gamma} \right)^{\dagger} \left( \frac{\partial \gamma}{\partial \gamma} \right) \right\}
\]
where the derivatives may be found as
\[
\frac{\partial x_{m,t}}{\partial \alpha_k} = \exp(ib_k)x_k^{m,t}, \quad \frac{\partial x_{m,t}}{\partial \beta_k} = -|t - \tau|\alpha_k x_k^{m,t},
\]
\[
\frac{\partial x_{m,t}}{\partial \omega_k} = i\alpha_k x_k^{m,t}, \quad \frac{\partial x_{m,t}}{\partial \eta_k} = -(t + 2\tau m)\alpha_k x_k^{m,t},
\]
\[
\frac{\partial x_{m,t}}{\partial \omega_k} = i\alpha_k x_k^{m,t}.
\]
Ruminent of the presentation in [7], these derivatives may be expressed on matrix form as \(\partial x_{m,\gamma}/\partial \gamma = Q_\alpha P\), where
\[
Q_m \triangleq \begin{bmatrix} \Xi_m \Theta & \Xi_m \Theta & \Xi_m \Theta & -\Xi_m \Theta & -\Xi_m \Theta \end{bmatrix}, \quad P \triangleq \text{diag} \left\{ [I \ A \ A \ A \ A] \right\} \in \mathbb{R}^{5K \times 5K},
\]
\[
\Xi_m \triangleq \begin{bmatrix} \xi_k^{m,t_0} & \cdots & \xi_k^{m,t_0} \\
\vdots & \ddots & \vdots \\
\xi_k^{m,N-1} & \cdots & \xi_k^{m,N-1} \end{bmatrix},
\]
\[
\Theta \triangleq \text{diag} \left\{ [e^{ib_1}, \ldots, e^{ib_K}] \right\},
\]
\[
A \triangleq \text{diag} \left\{ [a_1, \ldots, a_K] \right\}, \quad T \triangleq \text{diag} \left\{ [t_0, \ldots, t_{N-1}] \right\},
\]
\[
\dot{T} \triangleq \text{diag} \left\{ [t_0 - \tau, \cdots, t_{N-1} - \tau] \right\}, \quad \ddot{T} \triangleq \text{diag} \left\{ [(t_0 + 2\tau m), \cdots, (t_{N-1} + 2\tau m)] \right\}.
\]
Stacking the derivatives from each echo \(m\), yields \(\partial x/\partial \gamma = QP\), where
\[
Q = \begin{bmatrix} Q_T^{m} & \cdots & Q_T^{M-1} \end{bmatrix}^{T} \in \mathbb{C}^{NM \times 5K}.
\]

\begin{table}[]
\centering
\caption{Parameters for simulated data}
\begin{tabular}{|c|c|c|c|c|}
\hline
\(k\) & 1 & 2 & 3 & 4 \\
\hline
\(f_k\) (Hz) & 0.0329 & 0.0122 & 0.0049 & -0.0232 \\
\(\beta_k\) (Hz) & 0.0202 & 0.0077 & 0.0053 & 0.0035 \\
\(\eta_k\) (10^{-3}) & 0.1811 & 0.2647 & 0.2130 & 0.2221 \\
\(|\alpha_k|\) & 1.20 & 5.00 & 4.30 & 3.65 \\
\(\angle \alpha_k\) (rad) & 0.4591 & -2.8045 & 0.0661 & -1.9922 \\
\hline
\end{tabular}
\end{table}

The FIM thus becomes
\[
\text{FIM}(\gamma) = \frac{2}{\sigma^2} P \text{Re} \left\{ \left( Q^{H} Q \right) \right\} P
\]

implying that
\[
\text{CRB}(\gamma) = \frac{\sigma^2}{2} P^{-1} \left\{ \left( Q^{H} Q \right) \right\}^{-1} P^{-1}.
\]

Letting
\[
\Gamma \triangleq \left[ 2 \text{Re} \left\{ \left( Q^{H} Q \right) \right\} \right]^{-1}
\]

yields the further simplified expression for the sought CRBs
\[
\text{CRB}(\alpha_k) = \left[ t_k \alpha_k^2 / \text{SNR}_k \right],
\]
\[
\text{CRB}(\beta_k) = \left[ t_k (k+K)(k+2K) / \text{SNR}_k \right],
\]
\[
\text{CRB}(\omega_k) = \left[ t_k (k+2K)(k+4K) / \text{SNR}_k \right],
\]
\[
\text{CRB}(\eta_k) = \left[ t_k (k+4K)(k+6K) / \text{SNR}_k \right],
\]

where \(\text{SNR}_k = \alpha_k^2 / \sigma^2\).

4. NUMERICAL EXAMPLES

The proposed algorithm was evaluated using simulated NQR data, formed as to mimic the response signal from the explosive TNT when excited using a PSL sequence. Such signals can be well modeled as a sum of four damped sinusoidal signals, with the parameters as detailed in Table 1 (see [6] for further details on the signal and the relevant measurement setup). Based on the typical setup examined in [6], we use \(N = 256\) measurements, for \(M = 32\) echoes, with \(\tau = 164\) and \(f_0 = 36\), where the last two parameters are normalized with the sampling frequency and are therefore unit-less. The algorithm was evaluated using the normalized root mean squared error (NRMSE), defined as:
\[
\text{NRMSE} = \sqrt{\frac{1}{N} \sum_{p=1}^{N} \left( \frac{\hat{x}_p - x_p}{\sigma} \right)^2}
\]

where \(x_p\) denotes the true parameter value and \(\hat{x}_p\) the estimate of this parameter. The signal-to-noise ratio (SNR) is defined as \(\sigma_x^2 / \sigma^2\), with \(\sigma_x^2\) and \(\sigma^2\) denoting the power of the noise-free signal and the noise variance, respectively. Moreover, we use \(L = \hat{N} / 2\), where \(\hat{N}\) denotes the number of samples of either the expanding or the decaying part of the echo. With the used \(\tau\), one obtains a symmetric echo [6], so that \(L^{(+)} = L^{(-)} = 64\). Fig. 2 shows the results from \(P = 500\) Monte-Carlo simulations for the fourth spectral line (the performance for the other lines was similar). As is common for ESPRIT-based estimators, it can be noted that the ET-ESP estimate does not fully reach the CRB and is therefore not statistically efficient. However, the difference is very small down to \(\text{SNR} = 0\)
Fig. 2. NRMSE given by the proposed estimator for different parameters, compared with the respective CRB. Here, the NRMSE is empirically evaluated over 500 Monte-Carlo realizations, for symmetric echoes, with $N = 256$ and $M = 32$.

dB (which corresponds to $\sigma^2 \approx 6$), before which the estimation error becomes very large. For SNR = 5 dB, the estimation error for the frequency $f_4$ is about 0.2%, whereas for the damping coefficient, $\beta_4$, and the damping coefficient, $\eta_4$, it is about 8% and 3%, respectively. The amplitude error $|\alpha_4|$ is about 2%.

5. CONCLUSIONS

In this paper, we have derived an ESPRIT-based estimator and the corresponding CRB for the data model detailing the typically damped sinusoidal signals obtained in magnetic resonance measurements when formed using PSL data sequences. The estimator is computationally efficient and only requires the number of sinusoids to be known, which is typically the case in the considered applications. Via Monte-Carlo simulations, we have shown that the algorithm is close to being statistically efficient for typical signal-to-noise ratios. The proposed method offers an attractive alternative as a standalone estimator or as an initial estimator for further refined estimates based on gradient or search-based techniques.

6. REFERENCES


