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Multi-channel Detection of Narcotics and Explosives Using NQR Signals

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Abstract—A multi-channel detector for narcotics and explosives using nuclear quadrupole resonance (NQR) is developed. Multiple measurement coils are used to estimate the radio frequency interference that is often present. The temperature dependency of the NQR frequencies is incorporated in the detector, allowing for uncertainties in the temperature estimate of the sample. In addition, the detector considers only the frequency bands of the signal of interest.

I. INTRODUCTION

Nuclear quadrupole resonance (NQR) is a radio frequency (RF) technique offering an unequivocal method of detecting the presence of quadrupolar nuclei, such as the nitrogen isotope $^{14}$N, prevalent in many forms of high explosives, narcotics and drugs. Recently, the technique has received increasing attention as an important method for detecting land mines. This is because the NQR signal offers a unique signature, differentiating it from most other mine detection techniques that suffer from trying to detect non-unique features (such as the presence of metal). Figure 1 illustrates a typical example of an NQR signal, being well modeled as blocks of data from a sum of damped sinusoids. Further, NQR is also of particular interest due to the possibility of using the technique to detect explosives and/or narcotics at airports and other public places.

![Fig. 1. The real part of a typical echo train.](image)

Due to the used band of excitation frequencies, NQR signals are typically prone to strong RF interference (RFI), such as the ubiquitous AM radio transmissions present in the considered frequency band. In [1]–[3], various approximative maximum likelihood (AML) detectors were presented that exploited the fact that the shifts of the spectral lines depend in a known way on temperature. As an example, the shifting functions for monoclinic trinitrotoluene (TNT) are illustrated in Fig. 2. In general, these functions can be well modeled as

$$\omega_k(\tau) = a_k - b_k \tau$$

for known constants $a_k$ and $b_k$, with $\tau$ denoting the temperature of the examined sample. These detectors, that show both significant improvements in the probability of detection as compared to earlier detectors as well as robustness to residual RFI, are all formed from a single measurement antenna. In this paper, we further extend on these works, combining the efficient multi-channel RFI cancellation technique developed in [4], which assumes a fully known signal, with the structured
signal model suggested in [3].

Herein, as a way to reduce the sensitivity to the typical strong narrowband RFI, a frequency selective multi-channel (FSMC) detector is introduced. The FSMC detector operates only on a subset of the frequency grid, and it forms a weighted non-linear least squares estimate of the unknown parameters, using the combined response for these parameters as the detection variable.

II. THE MULTI-CHANNEL DATA MODEL

The $m$th echo of a single sensor noise-free NQR echo train, as illustrated in Fig. 1, can be well modeled as [3], [5]

$$x_{t,m} = \sum_{k=1}^{d} \alpha_k e^{-\eta_k(t)(t+m\mu)-\beta_k|t-t_{sp}|+iw_k(t)t}, \quad (2)$$

for $t = t_0, \ldots, t_{N-1}$, being the echo sampling time, with $N$ denoting the echo length, measured with respect to the center of the refocusing pulse, not necessarily being consecutive instances, but typically starting at $t_0 \neq 0$ to allow for the dead time between the pulse and the first measured sample (after the pulse). Furthermore, $\alpha_k$, $\beta_k$ and $\eta_k(t)$ denote the complex amplitude, the damping constant and the (temperature dependent) echo train damping function of the $k$th sinusoid, respectively; $\mu$ denotes the number of samples between the first sample of one echo and the first sample of the next echo, $t_{sp}$ is the known peak echo offset (due to the pulse spacing), and $w_k(t)$ is the frequency shifting function of the $k$th sinusoidal component due to the unknown temperature, $\tau$, of the observed sample. The relative ratio between the modulus of the signal amplitudes, $|\alpha_k|$, is often known for a given sample. Therefore, we let

$$\alpha_k = \rho \kappa_k, \quad (3)$$

where $\rho$ and $\kappa_k$ denote the common scaling constant due to the signal power, and the a priori known relative complex scalings between the $d$ signal components, respectively [1].

The frequency shifting function and the echo train damping function can be well modeled as (1) and

$$\eta_k(t) = c_k - d_k t, \quad (4)$$

respectively, where $c_k$ and $d_k$ are given constants (see [3], [5]–[7] for further details). We note that the herein presented detectors can easily be extended to also exploit multiple polymorphic forms along the lines discussed in [8]. Hereafter, to simplify the notation, we will omit the temperature dependence of $\omega_k(t)$ and $\eta_k(t)$, using only the notation $\omega_k$ and $\eta_k$.

Following [3], [5], let

$$x_m = \begin{bmatrix} x_{t_{0,m}} & \cdots & x_{t_{N-1,m}} \end{bmatrix}^T = \rho A_\theta \Psi_m, \quad (5)$$

where $A_\theta = B \odot P$, and

$$B = \begin{bmatrix} 1 & \cdots & 1 \\ \zeta_1 & \cdots & \zeta_d \\ \vdots & \cdots & \vdots \\ \zeta_1 & \cdots & \zeta_d \\ e^{-\beta_1(t_0-t_{sp})} & \cdots & e^{-\beta_d(t_0-t_{sp})} \\ e^{-\beta_1(t_1-t_{sp})} & \cdots & e^{-\beta_d(t_1-t_{sp})} \\ \vdots & \cdots & \vdots \\ e^{-\beta_1(t_{N-1}-t_{sp})} & \cdots & e^{-\beta_d(t_{N-1}-t_{sp})} \end{bmatrix}, \quad (6)$$

$$P = \begin{bmatrix} e^{-\eta_1} & \cdots & e^{-\eta_d} \\ \eta_1 & \cdots & \eta_d \end{bmatrix}, \quad (7)$$

$$\theta = \begin{bmatrix} \tau & \beta^T & \eta^T \end{bmatrix}^T, \quad (8)$$

$$\beta = \begin{bmatrix} \beta_1 & \cdots & \beta_d \end{bmatrix}^T, \quad (9)$$

$$\eta = \begin{bmatrix} \eta_1 & \cdots & \eta_d \end{bmatrix}^T, \quad (10)$$

$$\Psi_m = \begin{bmatrix} \kappa_1 e^{-\eta_1} & \cdots & \kappa_d e^{-\eta_d} \end{bmatrix}^T, \quad (11)$$

with $\zeta_k = e^{i\omega_k-\eta_k}$, and $(\cdot)^T$ and $\odot$ denoting the transpose and the Schur-Hadamard (element-wise) product, respectively. Using (5), an echo train consisting of $M$ echoes can be written as

$$x_m^T = \rho \vee [A_\theta \Lambda] \triangleq \rho z_\theta, \quad (12)$$

where the operation $\vee [X]$ stacks the columns of the matrix $X$ on top of each other, and

$$\Lambda \triangleq \begin{bmatrix} \Psi_0 & \cdots & \Psi_{M-1} \end{bmatrix}. \quad (13)$$

To reduce the influence of the noise and the RFI, $L$ multiple sensors can beneficially be used to measure the signal of interest, forming the measured signal

$$y_\ell = \rho a z_\theta(\ell) + w_\ell, \quad (14)$$

where $y_\ell \in \mathbb{C}^{L \times 1}, \ell = 0, \ldots, N M - 1$, denotes the array output at time index $\ell$, the array steering vector $a \in \mathbb{C}^{L \times 1}$ is known, $z_\theta(\ell)$ is the $\ell$th element of $z_\theta$, and $w_\ell \in \mathbb{C}^{L \times 1}$ is an additive noise and interference term. In general, the underlying thermal (Johnson) noise of each RF antenna may be well modeled as a temporally white noise process. However, the noise process will be shaped by the bandwidth of the receiver, due to the quality (Q) factor of the probe, and the settings (impulse response) of the anti-aliasing filter [1], [3]. To model this temporal noise shaping, we will herein use the approximative low order AR model derived in [1]. Furthermore, to allow for the spatial correlation between the sensors, we will model the additive noise process as a spatially colored circularly symmetric complex Gaussian process with unknown spatial covariance matrix $Q$.

III. THE FSMC DETECTOR

The temporally correlated noise sequence will be asymptotically (for large $N M$) uncorrelated on the Fourier grid [9]. As it is known that the signal of interest lies in a series of essentially known narrow bands of frequencies, one can beneficially derive a frequency selective detector which is formed from (only) these frequency bands.
Consider the frequency grid points
\[
\left\{ \frac{2\pi k_1}{N}, \ldots, \frac{2\pi k_M}{N} \right\}, \tag{15}
\]
with \(k_1, \ldots, k_M\) being \(M\) given, not necessarily consecutive, integers selected such that (15) only consists of the possible frequency grid points for each of the \(d\) signal components. Each such region is given by the minimal and maximal frequency values for that component considering the measured temperature and the size of the expected temperature uncertainty region. Denoting the measured temperature \(\hat{\tau}_m\), and the temperature uncertainty region \(\Delta_{\tau_m}\), we obtain the minimal and maximal frequency values using (1) with \(\tau = \hat{\tau}_m - \Delta_{\tau_m}\) and \(\tau = \hat{\tau}_m + \Delta_{\tau_m}\). It should be stressed that known interference sources, such as, for instance, radio broadcasts, can easily be excluded by omitting the frequency grid points of such carriers. This can be done even if these regions are part of the expected frequency regions of interest. The \(k\)th frequency grid point of the data matrix of the \(m\)th echo can be expressed as the 1 \(\times \) \(L\) vector
\[
f_k^m \triangleq v_k^T x_m a^T + E_k^m = \rho v_k^T \Psi_m a^T + E_k^m, \tag{16}
\]
where \(E_k^m = v_k^T W_m\), with \(W_m\) denoting the part of the additive noise affecting the \(m\)th echo, and
\[
v_k = \begin{bmatrix} 1 & z_k & \ldots & z_k^{N-1} \end{bmatrix}^T,
\tag{17}
\]
with \(z_k = e^{i2\pi k/N}\). The term \(E_k^m\) will (asymptotically) be a zero-mean temporally white but spatially colored circularly symmetric Gaussian process with unknown spatial covariance matrix \(Q_E\). It should be stressed that even though \(E_k^m\) will be (asymptotically) uncorrelated on the Fourier grid point [9], each of the frequency grid points will have a different variance, \(\sigma_{E_k}^2\). As shown in [1], the single-coil noise process, \(w(t)\), can be well modeled as a low order AR process,
\[
e(t) = C(z)w(t). \tag{18}
\]
As a result, it holds that
\[
\sigma_{E_k}^2 = \frac{\sigma^2}{|C(e^{i\omega_k})|^2}. \tag{19}
\]
Without loss of generality, we will here assume that \(\sigma^2 = 1\). We remark that the thus assumed noise model is a particular form of a multidimensional AR process; if needed, the proposed algorithm can easily be extended to handle also general multidimensional AR processes. Taking (19) into account, we form
\[
\hat{f}_k^m \triangleq \rho \sigma_{E_k}^{-1} f_k^m = \rho \sigma_{E_k}^{-1} v_k^T \Psi_m a^T + \hat{E}_k^m, \tag{20}
\]
where \(\hat{E}_k^m = \sigma_{E_k}^{-1} E_k^m\) is a zero-mean, unit variance, temporally white process with spatial covariance matrix \(Q_E\). Thus, over the (possibly overlapping) frequency regions of interest, (20) can be expressed as
\[
F_{M\hat{M}}^m = \rho V^* A \Psi_m a^T + G_{M\hat{M}}^m, \tag{21}
\]
where
\[
F_{M\hat{M}}^m = \begin{bmatrix} (f_{k_1}^m)^T & \ldots & (f_{k_M}^m)^T \end{bmatrix}^T, \tag{22}
\]
\[
G_{M\hat{M}}^m = \begin{bmatrix} (\hat{E}_{k_1}^m)^T & \ldots & (\hat{E}_{k_M}^m)^T \end{bmatrix}^T, \tag{23}
\]
\[
V_{M\hat{M}}^m = \begin{bmatrix} \sigma_{E_k}^{-1} v_k^m \ldots \sigma_{E_k}^{-1} v_k^m \end{bmatrix}^T. \tag{24}
\]
Using (21), the data model for the whole echo train can be expressed as,
\[
F_{M\hat{M}} \triangleq \begin{bmatrix} (F_0^m)^T & \ldots & (F_{M-1}^m)^T \end{bmatrix}^T \tag{25}
\]
\[
= \rho \text{vec} [V^* A \Lambda] a^T + G_{M\hat{M}} \tag{26}
\]
\[
= \rho \hat{z}_\theta a + G_{M\hat{M}}, \tag{27}
\]
where the \(M\hat{M} \times L\) matrix \(G_{M\hat{M}}\) is defined similar to \(F_{M\hat{M}}\).

Reordering (27) to write it in a form similar to (14), we introduce
\[
\hat{y}_\ell \triangleq [F_{M\hat{M}}^\ell]^T = \rho a \hat{z}_\theta(\ell) + \tilde{g}_\ell, \tag{28}
\]
for \(\ell = 0, \ldots, M\hat{M} - 1\), where \([X]_\ell\) denotes the \(\ell\)th column of \(X\), \(\hat{z}_\theta(\ell)\) is the \(\ell\)th element of \(\hat{z}_\theta\), and \(\tilde{g}_\ell = [G_{M\hat{M}}]^\ell\). Thus, the negative normalized log-likelihood function of the resulting sequence can be seen to be proportional to
\[
L_f = \log |Q_E| + \text{tr} \left\{ Q_E^{-1} Q_E \right\}, \tag{29}
\]
where \(|\cdot|\) and \(\text{tr}\{\cdot\}\) denote the determinant and the trace of a matrix, respectively. Minimization of \(L_f\) with respect to \(Q_E\) yields [10]
\[
\hat{Q}_E = \frac{1}{MM} \sum_{\ell=0}^{M\hat{M}-1} \left( \hat{y}_\ell - \rho a \hat{z}_\theta(\ell) \right) \left( \hat{y}_\ell - \rho a \hat{z}_\theta(\ell) \right)^*, \tag{30}
\]
and by inserting (30) into (29),
\[
L_f = \log |\hat{Q}_E| + L \tag{31}
\]
follows. The maximum likelihood estimate of \(\rho\), for a given \(\theta\), is then given as [4, 10]
\[
\hat{\rho} = \frac{a^* \hat{T}_\theta^{-1} \hat{f}_\theta}{P_\theta a^* \hat{T}_\theta^{-1} a}, \tag{32}
\]
where
\[
P_\theta = \hat{z}_\theta \hat{z}_\theta^*/(M\hat{M}), \tag{33}
\]
\[
T_\theta = \hat{R} - \hat{f}_\theta \hat{f}_\theta^*/P_\theta, \tag{34}
\]
\[
\hat{f}_\theta = \frac{1}{MM} \sum_{\ell=0}^{M\hat{M}-1} \hat{y}_\ell \hat{z}_\theta(\ell), \tag{35}
\]
\[
\hat{R} = \frac{1}{MM} \sum_{\ell=0}^{M\hat{M}-1} \hat{y}_\ell \hat{y}_\ell^*. \tag{36}
\]
Moreover, it can be shown that

\[ \hat{\theta} = \arg \max_\theta \frac{|a^* \hat{R}^{-1} \hat{f}_\theta|^2}{\left(1 - \hat{f}_\theta^* \hat{R}^{-1} \hat{f}_\theta\right) a^* \hat{R}^{-1} a + |a^* \hat{R}^{-1} \hat{f}_\theta|^2}, \tag{37} \]

where \( \hat{f}_\theta = \hat{f}_\theta \hat{R}^{-1/2} \).

The FSMC detector is now formed as

\[ \lambda_y \triangleq \log T_y = M \hat{M} \log |\hat{R}| - M \hat{M} \log |Q_{E, \hat{\theta}}|, \tag{38} \]

where \( T_y \) is an approximative generalized likelihood ratio test, \( \hat{\theta} \) is obtained as the parameter vector maximizing (37), and \( Q_{E, \hat{\theta}} \) is obtained by inserting the \( \theta \) maximizing (37) in (30).

As noted in [1]–[3], one can often, without significant loss in performance, use the approximations \( \beta_k \approx \beta_0 \) and \( \eta_k(\tau) \approx \eta_0 \), enabling the maximization in (37) to be approximated with the maximization over \( \{\tau, \beta, \eta_0\} \), being formed using three one-dimensional searches.\(^1\) Using (38), the signal component is deemed present if and only if \( \lambda_y > \gamma \), and otherwise not, where \( \gamma \) is a predetermined threshold value reflecting the acceptable probability of false alarm.

IV. NUMERICAL STUDIES

To illustrate the performance of the proposed detector using simulated multi-channel NQR data, a simulation model is formed from real single-channel NQR data measured from the high explosive TNT. The simulated data mimics a signal obtained using four solenoidal coils, where the first coil measures the signal of interest as well as interference and noise, while the other coils only measure interference and noise. Each coil allows for the estimation of \( M = 31 \) consecutive decaying echoes for every train of RF pulses, with each echo consisting of \( N = 256 \) data samples. The left part of Fig. IV shows the receiver-operator characteristic (ROC) curve for the alternating least squares (ALS) and the model-mismatched maximum likelihood (M3L) detectors, both presented in [4], and the proposed FSMC method, obtained using simulated interference-free NQR data, at a signal-to-noise ratio (SNR) of \(-36 \text{ dB}\), via 1000 Monte Carlo simulations. Here, the proposed approach allows for a temperature uncertainty region of \( \pm 10^3 \text{K} \) around the true temperature, as well as large search regions over the damping and echo damping constants (see [3] for details of the full data model). The matched filter technique assumes a known signal of interest, requiring perfect knowledge of the temperature of the explosive sample, as well as the set of damping and echo damping constants. Typically, it is difficult to estimate the temperature of a buried, or hidden, sample with more than \( 5^\circ \text{K} \) accuracy. As a comparison, we therefore also include the ROC curves for ALS and M3L for a \( 5^\circ \text{K} \) offset. As is clear from the figure, the proposed FSMC method offers robust detection schemes for cases when the temperature of the explosive sample is not fully known. We note that for signals without interference, the ALS and M3L detectors will coincide.

To examine the effects of common interference, we add a simplistic interference signal consisting of six sinusoids with zero mean Gaussian amplitude and frequencies uniformly distributed over the interval \([0, 2\pi]\). The right part of Fig. IV illustrates the ROC curves at a SNR of \(-36 \text{ dB}\). As is clear from the figure, the ALS and M3L detectors suffer a significant loss of detection performance due to the presence of the narrowband interference, whereas the FSMC is only mildly affected. The robustness of the FSMC detector is expected as it is formed over a set of limited frequency regions, and is therefore only affected by interference outside these regions via the FFT sidelobes. Also from this figure, we note that the FSMC detector, as it allows for an uncertainty in the temperature estimate, will be significantly more robust than the ALS and M3L detectors to such uncertainties.

\[^1\] As shown in [3], one can in cases where \( \eta_k(\tau) \) is not fully known, instead treat it as an unknown constant. In our experience, there is no significant performance loss in searching for this constant in place of using the actual shifting functions.
V. CONCLUSIONS

An efficient, robust, and frequency selective multi-channel detector to detect narcotics and explosives using NQR has been presented. The detector can handle significant uncertainties in the temperature estimate of the sample, since constructive use of the temperature dependency of the NQR frequencies are made.

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