

NON-PARAMETRIC DATA-DEPENDENT ESTIMATION OF SPECTROSCOPIC ECHO-TRAIN SIGNALS

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ABSTRACT

This paper proposes a novel non-parametric estimator for spectroscopic echo-train signals, termed ETCAPA, to be used as a robust and reliable first-approach-technique for new, unknown, or partly disturbed substances. Exploiting the complete echo structure for the signal of interest, the method reliably estimates all parameters of interest, enabling initial estimates for the identification procedure to follow. Extending the recent dCapon and dAPES algorithms, ETCAPA exploits a data-dependent filter-bank formulation together with a non-linear minimization to give a hitherto unobtained non-parametric estimate of the echo train decay. The proposed estimator is evaluated on both simulated and measured NQR signals, clearly showing the excellent performance of the method, even in the case of strong interferences.

Index Terms— Nuclear Quadrupole Resonance, echo-train signals, radio-frequency spectroscopy, non-parametric estimation, filter-bank methods.

1. INTRODUCTION

Nuclear quadrupole resonance (NQR) is a solid-state radio frequency (RF) technique that may be used to identify substances containing quadrupolar nuclei, such as found in many forms of explosives, narcotics, and medicines (see e.g., [1,2]). Measurements are commonly formed using so-called pulse lock sequences (PSL), wherein a train of RF pulses are transmitted at or close to the expected excitation frequency (or the dominant such frequency), generating a decaying echo train [3]. Figure 1 illustrates the envelope of the resulting echo-train (ET) data as obtained using a pulse spacing of τ . Typical analysis and detection algorithms for ET data requires some initial estimates of the expected echo decay within each echo, here denoted β , as well as the overall echo train decay, denoted η , capturing the decay over the various echoes [3, 4]. Such estimates are typically obtained using parametric estimators, such as the ET-ESPRIT and ETAML [3,5], or non-parametric data-adaptive estimators, such as the dCapon, dAPES, or dIAA algorithms [6,7]. The former kind of estimators suffer from requiring *a priori* knowledge of the precise data structure and model orders, including the presence of any possible interference components, which are commonly oc-

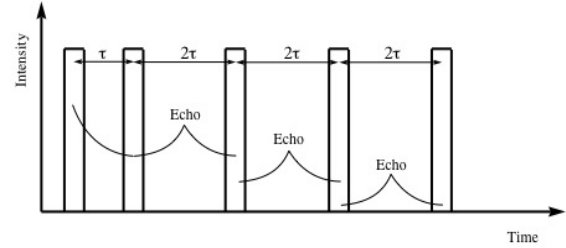


Fig. 1. The PSL sequence and corresponding NQR echo train signal. The β is here visual being the exponential decay in every echo and η as the decay between echoes.

curing in all forms of NQR measurements (see e.g., [4]). The mentioned non-parametric estimators on the other hand are robust to such assumptions, allowing for a spectral estimate enabling the separation of the NQR signal and the interference signals, but are then not able to estimate the finer structure of the ET, but rather just an overall exponential decay. In this paper, we extend on the methods in [6, 7], presenting a non-parametric data-dependent estimator of both the β and η decays of each relevant spectral line. In order to reduce the computational complexity of the method, the introduced ETCAPA estimator is formed in two steps, such that an initial estimate of the relevant frequencies using a simple exponential decay is formed by a combination of dCapon and dAPES, from which the (β, η) decays are then found for any frequency component of interest. The proposed method is evaluated on both simulated and measured data of the common high explosive TNT, as well as the narcotic methamphetamine.

2. DATA MODEL

As shown in [3], the m :th echo of the NQR signal resulting from a PSL sequence may be well modeled as

$$y(t, m) = \sum_{k=1}^K \alpha_k \lambda_k^t \rho_k^m + w(t, m), \quad t = 0 \dots N-1, \quad (1)$$

$$\lambda_k = e^{-\beta_k - \eta_k + i\omega_k},$$

$$\rho_k = e^{-2\tau\eta_k}$$

for echo $m = 0, \dots, M-1$, where τ is half the distance between two consecutive echoes, K is the number of spectral lines, ω_k denotes the k :th spectral line, β_k and η_k are the damping within each echo and the echo train damping, respectively, for spectral line k , and with $w(t, m)$ denoting an additive noise that is well modeled as being Gaussian distributed. To simplify notation, we have here, without loss of generality, treated the signal components formed from time τ in each echo, i.e., only considering the decaying part of each echo; the exploding part may be treated similarly, if present (this depends on the substance). The additive noise may typically be modeled using a low-order autoregressive model, reflecting the spectral shaping of the spectrometer [8]. Often, a number of strong but narrowband spurious peaks and interference components are also present due to poor or inadequate shielding of the examined sample, the equipment, or its wiring. In this work, we focus on non-parametric estimation of the β and η decays for each spectral line of interest, without making any assumptions on the model order of the signal.

3. THE ETCAPA ALGORITHM

Averaging the m echoes yields the averaged signal

$$x(t) = \sum_{m=0}^{M-1} \left\{ \sum_{k=1}^K \frac{1}{M} \alpha_k \lambda_k^t \rho_k^m + w(t) \right\} \quad (2)$$

$$= \sum_{k=1}^K \lambda_k^t \alpha_k \frac{1}{M} \sum_{m=0}^{M-1} \rho_k^m + e(t) \quad (3)$$

$$= \sum_{k=1}^K \lambda_k^t \tilde{\alpha}_k + e(t) \quad (4)$$

for $t = 1, \dots, N-1$, where $e(t)$ denotes the echo averaged noise and interference. It should be noted that the thus averaged interference components will, in general, be out of phase between the different echoes, thereby causing an improved *signal-to-interference-plus-noise ratio* (SINR) in the averaged signal, as compared to the full ET signal. It is also worth noting that the averaged amplitudes, $\tilde{\alpha}_k$, will be less or equal to α_k as

$$0 < \frac{1}{M} \sum_{m=0}^{M-1} \rho^m = \frac{1}{M} \sum_{m=0}^{M-1} e^{-2\tau\eta_k m} \leq 1 \quad (5)$$

Clearly, when averaging the echoes, the damping constants appearing in the exponent of λ will be combined, making it hard to separate them by just examining the averaged echo. Therefore, let γ denote the combined damping constant of a generic spectral line, such that

$$\gamma = \beta + \eta \quad (6)$$

Define a narrowband bandpass filter

$$\mathbf{h}_{\gamma, \omega} = [h_0 \quad \dots \quad h_{L-1}]^T \quad (7)$$

focused at frequency ω and the combined damping γ . Then, filtering the vector containing the L most recent samples of the averaged ET signal,

$$\mathbf{x}(t) = [x(t) \quad \dots \quad x(t+L-1)]^T \in \mathcal{C}^{L \times 1} \quad (8)$$

for $t = 0, \dots, N-L-1$, through $\mathbf{h}_{\gamma, \omega}$ yields

$$x^F(t) = \mathbf{h}_{\gamma, \omega}^* \mathbf{x}(t) \quad (9)$$

$$= [\mathbf{h}_{\gamma, \omega}^* \mathbf{a}_L(\gamma, \omega)] \tilde{\alpha} \lambda^t + e^F(t) \quad (10)$$

where $e^F(t)$ denotes the filtered noise component, and

$$\mathbf{a}_L(\gamma, \omega) = [1 \quad \dots \quad \lambda^{L-1}]^T \quad (11)$$

In order to ensure that the frequency and decay component of interest is passed undistorted, the filter is constrained so that

$$\mathbf{h}_{\gamma, \omega}^* \mathbf{a}_L(\gamma, \omega) = 1 \quad (12)$$

suggesting that filter focused at (γ, ω) minimizing the signal variance should be formed as

$$\begin{aligned} \mathbf{h}_{\gamma, \omega} &= \arg \min_{\mathbf{h}_{\gamma, \omega}} (\mathbf{h}_{\gamma, \omega}^* \hat{\mathbf{R}} \mathbf{h}_{\gamma, \omega}) \quad \text{subj. to (12)} \\ &= \frac{\hat{\mathbf{R}}^{-1} \mathbf{a}_L(\gamma, \omega)}{\mathbf{a}_L^*(\gamma, \omega) \hat{\mathbf{R}}^{-1} \mathbf{a}_L(\gamma, \omega)} \end{aligned} \quad (13)$$

with $\hat{\mathbf{R}}$ being a covariance estimate of $\mathbf{x}(t)$. In vector form, the resulting signal becomes

$$\mathbf{x}_{N-L}^F = \tilde{\alpha} \mathbf{a}_{N-L} + \mathbf{e}_{N-L}^F \quad (14)$$

where \mathbf{e}_{N-L}^F denotes a vector containing the $N-L$ most recent filtered noise components and \mathbf{a}_{N-L} analogously to (11). The amplitude estimate for the corresponding (γ, ω) component may then be formed using the least squares estimate

$$\hat{\alpha}(\gamma, \omega) = [\mathbf{a}_{N-L}^H \mathbf{a}_{N-L}]^{-1} \mathbf{a}_{N-L}^H \mathbf{x}_{N-L}^F \quad (15)$$

with the resulting $\hat{\alpha}(\gamma, \omega)$ estimate yielding a spectral surface over a pre-chosen 2-D grid, indicating the frequencies and combined dampings with notable power. In order to refine the estimates for these components, we propose forming a CAPES-like [10] estimate, refining the amplitude estimates of these components using dAPES [11]. The resulting amplitude estimates will be more accurate than the ones obtained by (15), and can then be used in a second refinement stage estimating the power distribution over β and η separately, for each notable component. By iterating the steps in (13)-(15) for every echo in the signal separately, M estimates of α_m are obtained, one for every echo, instead of only the averaged estimate obtained in (15). Denote $\hat{\alpha}(\gamma, \omega)$ the $(M \times 1)$ vector

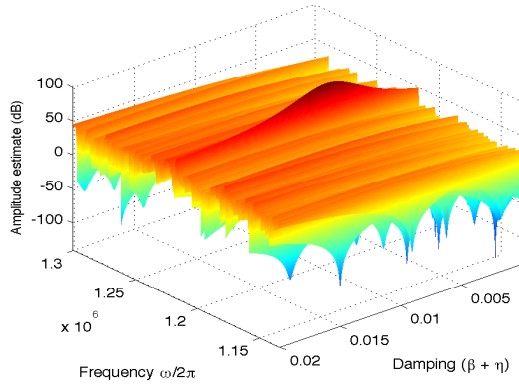


Fig. 2. The dCapon spectrum over frequency and total damping, γ , for an echo-averaged measured methamphetamine NQR signal with SNR = 5.8 dB.

containing these estimates. Redefining the complex amplitudes of echo m as $\alpha_m = \alpha \rho^m$, it follows then from the least squares estimation, and (14), that

$$\hat{\alpha}_m = \alpha \rho^m + \epsilon_m \quad (16)$$

If expressed in vector form,

$$\hat{\alpha} = \alpha \rho_\eta + \epsilon \quad (17)$$

where

$$\rho_\eta = [1 \quad \dots \quad \rho^{M-1}] \quad (18)$$

Then, minimizing the modeling error over the unknown α and η , such that

$$\{\alpha, \eta\} = \arg \min_{\alpha, \eta} \|\hat{\alpha} - \rho_\eta \alpha\|_2^2 \quad (19)$$

yields

$$\hat{\alpha} = (\rho_\eta^* \rho_\eta)^{-1} \rho_\eta^* \hat{\alpha} \quad (20)$$

which inserted in (19) results in

$$\hat{\eta} = \arg \min_{\eta} \hat{\alpha}^* \Pi_\rho^\perp \hat{\alpha} \quad (21)$$

where

$$\Pi_\rho^\perp = \mathbf{I} - \Pi_\rho = \mathbf{I} - \hat{\rho} \hat{\alpha} \quad (22)$$

denotes the projection onto the space orthogonal to ρ_η . The minimization in (21) may be calculated using standard gradient search techniques, e.g. using the Newton method, yielding the estimated echo train damping $\hat{\eta}$. The corresponding β estimate may then simply be obtained using (6), as

$$\hat{\beta} = \hat{\gamma} - \hat{\eta} \quad (23)$$

Finally, the corresponding amplitude estimate for this component, α , may easily be re-estimated by either inserting $\hat{\eta}$ in (4), or by using the least squares estimate derived above.

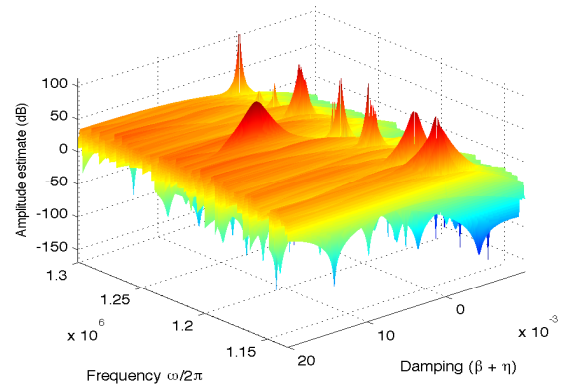


Fig. 3. The dCapon spectrum for an echo-averaged experimentally realistic methamphetamine NQR signal corrupted by sinusoidal interference.

4. NUMERICAL RESULTS

We proceed to examine the accuracy of the proposed estimator using methamphetamine measurements performed on seizures by the Japanese customs, formed on $M = 15$ echoes with $N = 295$ samples each. This data set is estimated to have a *signal-to-noise ratio* (SNR) of 5.8 dB, where SNR is defined as

$$\text{SNR} = 10 \cdot \log \left(\frac{P_{\text{signal}}}{P_{\text{noise}}} \right) \quad (\text{dB}) \quad (24)$$

and $P_{(\cdot)}$ is the power of respective signal type. Figure 2 shows the dCapon spectral estimate of the (γ, ω) surface for the averaged signal $x(t)$, which if forming the ETCAPA estimate obtained using (15), (19), (21), and (23), for its spectral peak of interest, yields

$$\begin{aligned} \hat{\theta}_{\text{ETCAPA}} &= [\hat{f} \quad \hat{\beta} \quad \hat{\eta}] \\ &= [-0.0001 \quad 0.00578 \quad 0.001921] \end{aligned} \quad (25)$$

where $f = \omega/2\pi$. This can be compared to the parametric estimate obtained by the ETAML algorithm [8], yielding

$$\hat{\theta}_{\text{ETAML}} = [-0.00016 \quad 0.00543 \quad 0.001927] \quad (26)$$

indicating a similar accuracy for both the parametric and non-parametric estimators. The difference in the estimation of frequency is due to the used grid size, which is not the case for β and η . The difference in these estimates as compared to the ETAML estimates can likely be explained by the fact that the measured NQR signals will not be corrupted by an white additive noise, and even though the ETAML algorithm exploits a low-order AR approximation of this noise, it will likely yield estimates that are somewhat biased. In order to clarify this, we proceed to examine simulated data, considering the multi-line region of a sample of TNT (see [8] for

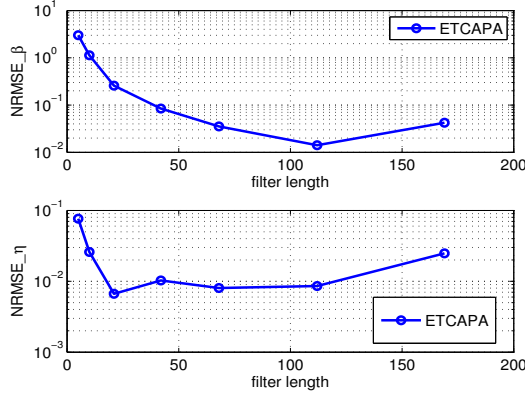


Fig. 4. NRMSE estimations over different values of filter length. A minimum error is reached around 110, which is about $N/3$.

details this data set). Table 1 shows the resulting estimation errors for the ETCAPA estimates, using $M = 32$ echoes with $N = 295$ samples each, with SNR = 10 dB, showing that the resulting errors can be considered to lie close to the grid spacing, which is $5 \cdot 10^{-4}$ over frequency and $0.5 \cdot 10^{-4}$ over β . Finally, we examine a simulated data set mimicking the earlier methamphetamine measurements, but now corrupted by several strong RFI components, 40 dB stronger than the studied NQR signal. Such very strong RFI components often occurs in non-shielded NQR measurements, but will due to the averaging of echoes influence the estimate less than could be expected. This can be seen in Figure 3, which clearly shows how the interference signals are weakened due to the averaging, thereby not disturbing the spectral estimate of the signal of interest. In this case, the strong interference components will corrupt the ETAML estimates, making them meaningless, whereas the ETCAPA estimates are almost as accurate as the ones obtained if no interference was present, being just above the level of the grid spacing. It is worth noting that except for defining a search grid over frequency and damping in the initial dCapon estimate, one also has to choose the length of the filters in (10). The performance of the estimator will be relatively insensitive to this choice, as shown in Figure 4, illustrating the normalized root mean error for the parameters β and η , as obtained using 500 Monte-Carlo simulations, for a SNR = 10 dB, for varying the filter lengths. The figure suggests that an appropriate should be set as $\text{floor}(N/3)$, where N is the number of samples. This is also how the filter length has been selected in the simulations above. It should be noted that the spectral lines for the considered cases will lie somewhat off the used spectral grid, indicating the typical robustness to the the assumption that the grid coincides with the true parameters (see also the related discussion in [12, 13]).

Table 1. Error estimates of frequencies and dampings for the $K = 4$ NQR components of monoclinic TNT.

k	1	2	3	4
$\Delta f_k \times 10^{-5}$	-4.9	5.0	3.7	11.5
$\Delta \beta_k \times 10^{-5}$	67	36	11	-17.5
$\Delta \eta_k \times 10^{-5}$	9.0	-0.9	0.12	-0.25

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