ON THE RECONSTRUCTION OF GAPPED SINUSOIDAL DATA

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ABSTRACT

The problem of estimating a spectral representation of damped sinusoidal signals from a gapped data set is of considerable interest in several applications. In this paper, we propose a filterbank approach to provide such an estimate, by first reconstructing the missing data samples assuming that the spectral content of the missing data is similar to that of the available samples, and then forming a spectral representation of the reconstrucéd data set as a function of frequency and damping. Numerical examples illustrate the benefits of the proposed estimator as compared to currently available methods.

***Index Terms*—** Spectral estimation, missing data, damped sinusoids

1. INTRODUCTION

Spectral analysis is a classical problem, finding application in a wide variety of fields, e.g., astronomy, communications, economics, medical imaging, and radar; consequently, there is a wealth of research pertaining to the problem (see, e.g., [1] and the references therein). The majority of the work focuses on estimating the spectrum from a finite sequence consisting of evenly sampled data. The amplitude and phase estimation (APES) algorithm is a good example of a high-quality algorithm that can be applied to such data [2]. In many applications, however, it is often not possible to sample the data evenly, leading to data sets which may be viewed as an evenly sampled data sequence in which samples are missing. The problem of estimating spectra when data is missing has been considered, e.g., in the astronomical literature, and several parametric and non-parametric methods have been proposed [3, 4]. Commonly, most methods first interpolate the missing data to yield a full data sequence without missing samples, on which ordinary spectral estimation algorithms may then be applied. In performing the interpolation, one is required to make assumptions on the missing data, which can be viewed as adding in extra information; therefore, such assumptions are of critical importance. The approach taken in [3] is particularly appealing, since the only assumption made is that the spectral content of the missing data is similar to that of the available data. Studies of this method, termed gapped-data APES (GAPES), illustrate the benefits of this approach [3, 4]. The problem of estimating the spectral parameters of damped sinusoidal data has recently attracted attention, since such signals arise naturally in several areas of spectroscopy, e.g., in nuclear magnetic resonance (NMR) and nuclear quadrupolar resonance (NQR). For instance, in [5], the damped APES (dAPES) algorithm was proposed to estimate spectra from the resulting data sets. Specifically, it is the free induction decay (FID) signal, measured using these spectroscopic methods, that may be well modeled as a sum of exponentially damped sinusoids. Obtaining purer FID signals is of significant interest in these applications and therefore new methods for acquiring FIDs are continuously investigated. One such method is stochastic excitation, which has found application in NMR [6, 7], electron paramagnetic resonance (EPR) [8] and NQR [9–11]. In many cases, the noise-free signal resulting from a stochastic excitation experiment can be well modeled as a *gapped* damped sinusoidal signal. In this paper, we focus on estimating the spectral representation of such data sets. Specifically, we combine the GAPES and dAPES algorithms to produce the damped GAPES (dGAPES) algorithm.

In the following, $(\cdot)^T$ and $(\cdot)^*$ denote the transpose and the conjugate transpose, respectively.

2. PRELIMINARIES

For completeness, we initially review the dAPES method for estimating the parameters of damped sinusoids [5]. Using this framework, we then extend the approach to also allow for the case of gapped data sequences.

When the entire data set is available, we can form the *complete* data vector, $\boldsymbol{y}$, as

$$\begin{aligned} \boldsymbol{y} &= \begin{bmatrix} y(0) & \cdots & y(N-1) \end{bmatrix}^T & (1) \\ &\triangleq \begin{bmatrix} \boldsymbol{y}_1^T & \boldsymbol{y}_2^T & \cdots & \boldsymbol{y}_P^T \end{bmatrix}^T, & (2) \end{aligned}$$

where $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_P$ are (non-overlapping) subvectors of $\boldsymbol{y}$, with lengths $N_1, \ldots, N_P$, respectively, such that $\sum_{p=1}^{P} N_p = N$. The dAPES spectral estimate can be interpreted as the output of an M-tap data dependent finite impulse response (FIR) filter with taps [1, 5]

$$\boldsymbol{h}_{\alpha,\omega} = \begin{bmatrix} h_0(\alpha,\omega) & h_1(\alpha,\omega) & \cdots & h_{M-1}(\alpha,\omega) \end{bmatrix}^T, \quad (3)$$

designed such that

1. the damped sinusoid $\{e^{(-\alpha+i\omega)t}\}$ passes undistorted through the filter;
2. the filter output is as close as possible in the least-squares (LS) sense to a damped sinusoid.

Thus, the output of the filter $\boldsymbol{h}_{\alpha,\omega}$, for generic values of the damping, α, and the frequency, ω, can be written as

$$\boldsymbol{h}^*_{\alpha,\omega}\bar{\boldsymbol{y}} = \rho_{\alpha,\omega} e^{-\alpha l + i\omega l} + w(t), \quad (4)$$

where ρ is the complex amplitude, and, for $l = 0, \ldots, L-1$,

$$\bar{\boldsymbol{y}}_l = \begin{bmatrix} y(l) & y(l+1) & \cdots & y(l+M-1) \end{bmatrix}^T, \quad (5)$$

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are the overlapping (forward) data snapshot vectors of dimension $(M \times 1)$, with $L = N - M + 1$, and $w(t)$ denotes the residual term containing the signal resulting from all frequencies and dampings different from α and ω. In order to minimize the residual term, the filter is designed as [5]

$$\min_{\rho(\alpha,\omega),\boldsymbol{h}_{\alpha,\omega}} \sum_{l=0}^{L-1} \left| \boldsymbol{h}_{\alpha,\omega}^* \bar{\boldsymbol{y}}_l - \rho_{\alpha,\omega} e^{-\alpha l + i\omega l} \right|^2 \quad \text{s.t.} \quad \boldsymbol{h}_{\alpha,\omega}^* \boldsymbol{s}_{\alpha,\omega} = 1, \tag{6}$$

where

$$\boldsymbol{s}_{\alpha,\omega} = \begin{bmatrix} 1 & e^{-\alpha+i\omega} & \cdots & e^{(-\alpha+i\omega)(M-1)} \end{bmatrix}^T. \tag{7}$$

Let

$$\hat{\boldsymbol{R}}_\alpha = \frac{1}{G(\alpha)} \sum_{l=0}^{L-1} \bar{\boldsymbol{y}}_l \bar{\boldsymbol{y}}_l^* \tag{8}$$

$$\bar{\boldsymbol{g}}_{\alpha,\omega} = \frac{1}{G(\alpha)} \sum_{l=0}^{L-1} \left[\bar{\boldsymbol{y}}_l e^{-\alpha l} \right] e^{-i\omega l}, \tag{9}$$

where

$$G_\alpha = \sum_{l=0}^{L-1} e^{-2\alpha l} = e^{-2\alpha} \frac{e^{-2\alpha L} - 1}{e^{-2\alpha} - 1}. \tag{10}$$

Then, the design objective (6), can be reformulated as [5]

$$\min_{\rho_{\alpha,\omega},\boldsymbol{h}_{\alpha,\omega}} G_\alpha \left[\left| \rho_{\alpha,\omega} - \boldsymbol{h}_{\alpha,\omega}^* \bar{\boldsymbol{g}}_{\alpha,\omega} \right|^2 + \boldsymbol{h}_{\alpha,\omega}^* \hat{\boldsymbol{Q}}_{\alpha,\omega} \boldsymbol{h}_{\alpha,\omega} \right] \quad \text{s.t.} \quad \boldsymbol{h}_{\alpha,\omega}^* \boldsymbol{s}_{\alpha,\omega} = 1, \tag{11}$$

where

$$\hat{\boldsymbol{Q}}_{\alpha,\omega} \triangleq \hat{\boldsymbol{R}}_\alpha - \bar{\boldsymbol{g}}_{\alpha,\omega} \bar{\boldsymbol{g}}_{\alpha,\omega}^*. \tag{12}$$

Minimizing (11) with respect to $\rho_{\alpha,\omega}$, yields

$$\hat{\rho}_{\alpha,\omega} = \boldsymbol{h}_{\alpha,\omega}^* \bar{\boldsymbol{g}}_{\alpha,\omega}, \tag{13}$$

which, when inserted in (11), yields

$$\min_{\boldsymbol{h}_{\alpha,\omega}} \boldsymbol{h}_{\alpha,\omega}^* \hat{\boldsymbol{Q}}_{\alpha,\omega} \boldsymbol{h}_{\alpha,\omega} \quad \text{s.t.} \quad \boldsymbol{h}_{\alpha,\omega}^* \boldsymbol{s}_{\alpha,\omega} = 1. \tag{14}$$

The solution to (14) is given by (see, e.g., [1])

$$\hat{\boldsymbol{h}}_{\alpha,\omega} = \frac{\hat{\boldsymbol{Q}}_{\alpha,\omega}^{-1} \boldsymbol{s}_{\alpha,\omega}}{\boldsymbol{s}_{\alpha,\omega}^* \hat{\boldsymbol{Q}}_{\alpha,\omega}^{-1} \boldsymbol{s}_{\alpha,\omega}}, \tag{15}$$

implying

$$\hat{\rho}_{\alpha,\omega} = \hat{\boldsymbol{h}}_{\alpha,\omega}^* \bar{\boldsymbol{g}}_{\alpha,\omega} = \frac{\boldsymbol{s}_{\alpha,\omega}^* \hat{\boldsymbol{Q}}_{\alpha,\omega}^{-1} \bar{\boldsymbol{g}}_{\alpha,\omega}}{\boldsymbol{s}_{\alpha,\omega}^* \hat{\boldsymbol{Q}}_{\alpha,\omega}^{-1} \boldsymbol{s}_{\alpha,\omega}}, \tag{16}$$

which allows for a two-dimensional spectral representation over both frequency and damping. As observed in [5], this representation has the significant benefit of allowing for separation of spectral peaks closely spaced in frequency but having different dampings, or vice versa, being of great interest in applications such as, e.g., NMR. We remark that direct evaluation of (15) is computationally intensive, as a matrix inverse is required for *every* considered α and ω. However, by exploiting the inherent structure of the filter, one may evaluate (15) in a computationally efficient manner [12].

3. NON-PARAMETRIC SPECTRAL ESTIMATION OF GAPPED DATA

We now proceed to allow for the case when some segments of the data are unavailable. These missing samples form the vector of *unavailable* data,

$$\boldsymbol{\mu} \triangleq \begin{bmatrix} \boldsymbol{y}_2^T & \boldsymbol{y}_4^T & \cdots & \boldsymbol{y}_{P-1}^T \end{bmatrix} \in \mathbb{C}^{(N-g)\times 1}. \tag{17}$$

Similarly, we form the vector of *available* data,

$$\boldsymbol{\gamma} \triangleq \begin{bmatrix} \boldsymbol{y}_1^T & \boldsymbol{y}_3^T & \cdots & \boldsymbol{y}_P^T \end{bmatrix} \in \mathbb{C}^{g\times 1}, \tag{18}$$

where $g = N_1 + N_3 + \ldots + N_P$ is the total number of samples available. We note that some of these sets may be empty, e.g., $N_3 = N_7 = 0$. Here, without loss of generality, P is assumed to be an odd number. Reminiscent of the GAPES method [3, 4], we proceed to formulate the proposed dGAPES estimator by:

1. Estimating the adaptive filter, $\boldsymbol{h}_{\alpha,\omega}$, and the corresponding spectrum, $\rho_{\alpha,\omega}$ via dAPES, and,
2. reconstructing the missing samples via an LS fit.

We now proceed to examine these two steps in further detail. First, we need to form initial dAPES estimates of $\boldsymbol{h}_{\alpha,\omega}$ and $\rho_{\alpha,\omega}$ from the available data. The filter length M_0 is chosen so that an initial full-rank matrix $\hat{\boldsymbol{R}}_\alpha$ can be built using only the *available* data segments. Then,

$$\sum_{p\in\{1,3,\ldots,P\}} \max(0, L_p) > M_0 \tag{19}$$

with $L_p = N_p - M_0 + 1$. Let $\mathcal{J}$ denote the subset of $\{1, 3, \ldots, P\}$ for which $L_p > 0$. Letting $\psi_p = N_1 + N_2 + \ldots + N_{p-1}$ denote the number of samples in the $p - 1$ first blocks, we redefine $\boldsymbol{R}_\alpha$ and $\bar{\boldsymbol{g}}_{\alpha,\omega}$ as

$$\hat{\boldsymbol{R}}_\alpha = \frac{1}{G_\alpha} \sum_{p\in\mathcal{J}} \sum_{l=\psi_p}^{\psi_p+L_p-1} \bar{\boldsymbol{y}}_l \bar{\boldsymbol{y}}_l^* \tag{20}$$

and

$$\bar{\boldsymbol{g}}_{\alpha,\omega} = \frac{1}{G_\alpha} \sum_{p\in\mathcal{J}} \sum_{l=\psi_p}^{\psi_p+L_p-1} [\bar{\boldsymbol{y}}_l e^{-\alpha l}] e^{-i\omega l} \tag{21}$$

so that the initial estimate of the dAPES filterbank in (15) uses only the available samples. Then, we use (16) to form an initial estimate of the amplitudes, where (9) is replaced by (21). Note that the data snapshots used in (20) and (21) are of dimensions $(M_0 \times 1)$ with elements only from the available data vector, $\boldsymbol{\gamma}$, defined in (18). We next turn to estimating the missing data, $\boldsymbol{\mu}$, defined in (17), based on the initial spectral estimates of $\hat{\rho}_{\alpha,\omega}$ and $\hat{\boldsymbol{h}}_{\alpha,\omega}$. We base our estimate on the assumption that the missing samples have the same spectral content as the available data. Thus, we estimate the missing data by fitting it as close as possible in the LS-sense to $\hat{\rho}_{\alpha,\omega} e^{(-\alpha+i\omega)l}$. By evaluating the estimates over K frequency points and D damping points, we can obtain $\boldsymbol{\mu}$ as the solution to the LS-problem

$$\min_{\boldsymbol{\mu}} \sum_{d=0}^{D-1} \sum_{k=0}^{K-1} \sum_{l=0}^{L-1} \left| \hat{\boldsymbol{h}}_{\alpha_d,\omega_k}^* \bar{\boldsymbol{y}}_l - \hat{\rho}_{\alpha_d,\omega_k} e^{(-\alpha_d+i\omega_k)l} \right|^2. \tag{22}$$

Define

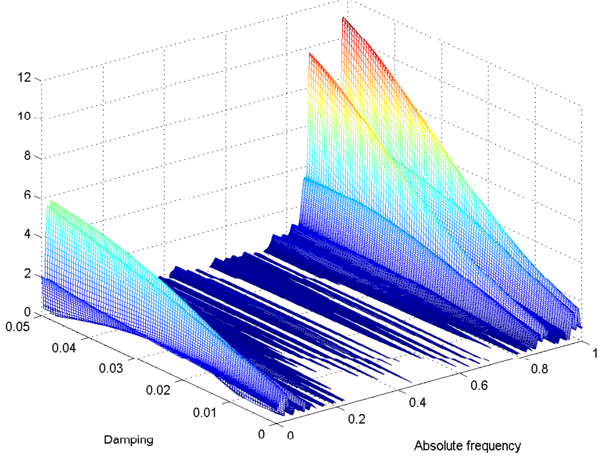

Fig. 1. The dCapon spectrum of original data.

$$\boldsymbol{H}_{d,k} \triangleq \begin{bmatrix} \hat{\boldsymbol{h}}^*_{\alpha_d,\omega_k} & & & \\ & \hat{\boldsymbol{h}}^*_{\alpha_d,\omega_k} & & \\ & & \ddots & \\ & & & \hat{\boldsymbol{h}}^*_{\alpha_d,\omega_k} \end{bmatrix} \in \mathbb{C}^{L\times N} \quad (23)$$

and

$$\boldsymbol{\eta}_{d,k} \triangleq \hat{\rho}_{\alpha_d,\omega_k} \begin{bmatrix} 1 \\ e^{-\alpha_d+i\omega_k} \\ \vdots \\ e^{(-\alpha_d+i\omega_k)(L-1)} \end{bmatrix}. \quad (24)$$

Using (23)-(24), one can rewrite (22) as

$$\sum_{d=0}^{D-1}\sum_{k=0}^{K-1} \left\| \boldsymbol{H}_{d,k}\boldsymbol{y} - \boldsymbol{\eta}_{d,k} \right\|^2. \quad (25)$$

Introducing the matrices $\boldsymbol{A}_{d,k} \in \mathbb{C}^{L\times g}$ and $\boldsymbol{U}_{d,k} \in \mathbb{C}^{L\times(N-g)}$, defined by

$$\boldsymbol{H}_{d,k}\boldsymbol{y} = \boldsymbol{A}_{d,k}\boldsymbol{\gamma} + \boldsymbol{U}_{d,k}\boldsymbol{\mu}, \quad (26)$$

allows (25) to be rewritten as

$$\sum_{d=0}^{D-1}\sum_{k=0}^{K-1} \left\| \boldsymbol{U}_{d,k}\boldsymbol{\mu} - (\boldsymbol{\eta}_{d,k} - \boldsymbol{A}_{d,k}\boldsymbol{\gamma}) \right\|^2. \quad (27)$$

An estimate of the missing data is thus the minimizer of (27) w.r.t. $\boldsymbol{\mu}$, i.e.,

$$\hat{\boldsymbol{\mu}} = \Upsilon_0^{-1} \sum_{d=0}^{D-1}\sum_{k=0}^{K-1} \boldsymbol{U}^*_{d,k}\left(\boldsymbol{\eta}_{d,k} - \boldsymbol{A}_{d,k}\boldsymbol{\gamma}\right), \quad (28)$$

where

$$\Upsilon_0 \triangleq \sum_{d=0}^{D-1}\sum_{k=0}^{K-1} \boldsymbol{U}^*_{d,k}\boldsymbol{U}_{d,k}. \quad (29)$$

Summarizing the algorithm, we note that once we have an estimate of the missing sample vector, $\hat{\boldsymbol{\mu}}$, we can use it, together with the available samples, to reestimate $\{\rho_{\alpha_d,\omega_k}, \boldsymbol{h}_{\alpha_d,\omega_k}\}_{k=0,d=0}^{K-1,D-1}$ from the available samples and the estimate of the missing samples. The problem of estimating the spectrum of gapped-data with damped sinusoids can hence be turned into a cyclic minimization problem of the form

$$\min_{\boldsymbol{\mu},\{\rho_{\alpha_d,\omega_k},\boldsymbol{h}_{\alpha_d,\omega_k}\}} \sum_{d=0}^{D-1}\sum_{k=0}^{K-1}\sum_{l=0}^{L-1} \Big| \boldsymbol{h}^*_{\alpha_d,\omega_k}\bar{\boldsymbol{y}}_l - \rho_{\alpha_d,\omega_k} e^{(-\alpha_d+j\omega_k)l} \Big|^2. \quad (30)$$

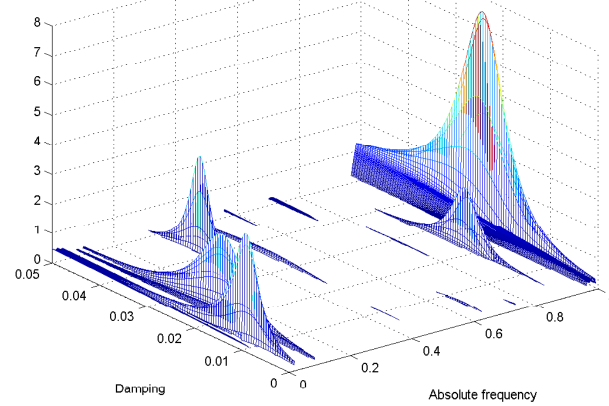

Fig. 2. The dCapon spectrum of data reconstructed using the dGAPES method.

In summary, the dGAPES algorithm consists of the following steps:

Step 0. Obtain an initial estimate of $\{\rho_{\alpha_d,\omega_k}, \boldsymbol{h}_{\alpha_d,\omega_k}\}$ from (15) and (16) using the available data.

Step 1. Use the most recent estimate of $\{\rho_{\alpha_d,\omega_k}, \boldsymbol{h}_{\alpha_d,\omega_k}\}$ to estimate $\boldsymbol{\mu}$, given by (28).

Step 2. Use the most recent estimate of $\boldsymbol{\mu}$ to fill in the missing data samples and estimate $\{\rho_{\alpha_d,\omega_k}, \boldsymbol{h}_{\alpha_d,\omega_k}\}$ by minimizing (30).

Step 3. Repeat steps 1-2 until practical convergence, e.g., until the relative change between the current and previous iteration of the cost function (30) is smaller than a fixed threshold ϵ.

We note that for increased resolution, it is possible to evaluate the spectral estimate on a finer damping and frequency grid when generating the amplitude estimates in the final iteration. We also note that the dGAPES method will generate a reconstructed set of data that can be used by other estimators, such as damped Capon (dCapon), damped CAPES (dCAPES) [5], or HTLS [13].

4. NUMERICAL EXAMPLES

To illustrate the benefits of the proposed algorithm, we examine stochastically excited NQR (sNQR) data mimicking the response from the explosive TNT. This data can be well modeled as a sum of five damped sinusoids [10, 11]. See Table 1 for parameters detailing the simulated sinusoids (see also [10, 11] for a more detailed model of the NQR response). Here, we generate an FID of length $N = 96$ samples, where we assume samples 33-64 were missing. This gives two blocks of available data, each of length 32. The data were corrupted by zero-mean circularly symmetric complex white Gaussian noise with power σ_w^2. We used a signal-to-noise ratio

Table 1. Estimates of the sNQR parameters for monoclinic TNT (k denotes the peak number)

k	1	2	3	4	5
ω_k (rad/s)	1.93	0.62	0.11	-0.089	-0.78
α_k (1e-2)	4.01	1.28	1.22	1.92	2.07
$\lvert\rho_k\rvert$	5.64	2.98	6.83	12.16	9.73
$\angle\rho_k$ (rad)	-0.17	2.52	-2.71	-2.29	-0.70

Table 2. MSE of S-HTLS, using the available-only data, and of HTLS, using the reconstructed data

Method	MSE		
	Amplitude	Frequency	Damping
S-HTLS	3.8433	3.675e-6	1.506e-4
HTLS	0.9599	1.667e-6	0.573e-4

(SNR) of 20 dB, where SNR is defined as SNR = $\sigma_w^{-2}\sigma_s^2$, with σ_s^2 denoting the power of the noise-free signal. For the initialization phase, we used a filter of length $M_0 = 12$, and in the other steps $M = 38$. For the computation, we used a frequency grid with $K = 512$ points, a damping grid with 101 equally spaced points in the interval $[0, 0.05]$, and an iteration threshold $\epsilon = 0.03$. Fig. 1 illustrates the dCapon spectral estimate of the available-only data set. We used the same damping grid as in the interpolation phase but with a finer frequency grid, i.e., $K = 2048$. As a comparison, Fig. 2 shows the dCapon spectral estimate of the reconstructed data set, using the same damping and frequency grid. The figures clearly illustrate the benefits of following the dGAPES approach which allows for a significantly higher resolution (in both frequency and damping) as compared to current state-of-the art techniques. We proceed to examine the gain in performance using the proposed dGAPES algorithm as compared to estimating the unknown parameters on the available data set. Table 2 shows the mean squared error (MSE) of the amplitudes, frequencies, and dampings, computed via the S-HTLS method [14], that uses only the available data, and the MSE computed via HTLS [13], using the reconstructed data. Here, the data was evaluated empirically using 1000 Monte-Carlo simulations. From the table, it is clear that using the reconstructed data allows for a substantial improvement of the parameter estimates.

5. CONCLUSIONS

In this paper, we have derived a method for estimation of the spectral representation of gapped damped sinusoidal data. Using only the natural assumption that the spectral content of the missing data is similar to that of the available data, we can interpolate to reconstruct the missing samples. From the reconstructed data we can then efficiently estimate the spectral content of the data, using any method, e.g., dCapon, dCAPES, HTLS, etc.

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