

Computationally Efficient Estimation of Multi-dimensional Damped Modes using Sparse Wideband Dictionaries*

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Abstract—Estimating the parameters of non-uniformly sampled multi-dimensional damped modes is computationally cumbersome, especially if the model order of the signal is not assumed to be known a priori. In this work, we examine the possibility of using the recently introduced wideband dictionary framework to formulate a computationally efficient estimator that iteratively refines the estimates of the candidate frequency and damping coefficients for each component. The proposed wideband dictionary allows for the use of a coarse initial grid without increasing the risk of not identifying closely spaced components, resulting in a substantial reduction in computational complexity. The performance of the proposed method is illustrated using both simulated and real spectroscopy data, clearly showing the improved performance as compared to previous techniques.

Index Terms—Sparse signal analysis, dictionary learning, damped sinusoids, wideband dictionaries

I. INTRODUCTION

Parameter estimation of high-dimensional damped modes is a topic of interest in a variety of fields, including spectroscopy, geology, sonar, and radar, and has as a result attracted notable interest in the literature (see, e.g. [1]–[7]). Common estimation approaches include subspace-based algorithms, such as the ones introduced in [1]–[3], and sparse framework techniques reformulating the estimation into a convex optimization problem (see, e.g., [6], [7]). The former approaches generally suffer from requiring detailed model knowledge, including accurate specification of the model order, often making them less robust to cases when such assumptions are violated. On the other hand, many common sparse techniques will suffer from the fact that exponentially decaying sinusoids do not have a sparse representation in oversampled Fourier matrices, typically necessitating an iterative zooming procedure over multiple dimensions. In [6], this was done by expanding the dictionary over a grid of frequency and damping candidates. However, such an approach suffers from high computational complexity and sub-optimal performance, typically requiring an accurate initialization or model order information to yield reliable results, information which is commonly not available in many of the discussed applications. To alleviate this problem, we recently introduced a framework that iteratively refines the estimates of the candidate frequency and damping coefficients for each component [7], thus allowing for smaller dictionaries, as well as for frequency and damping parameters that are not restricted to a pre-defined grid. In [7], we further

introduced a Kronecker structure based implementation which, although being efficient for the case of uniformly sampled data, does not allow for arbitrary non-uniform sampling patterns.

However, non-uniform sampling is often of particular interest for high-dimensional problems, where the data may be measured in so-called indirect dimensions. This is, for example, the case in nuclear magnetic resonance (NMR) spectroscopy, wherein one measures the free induction decay (FID) resulting from pulsing a substance of interest. By varying the pulse settings, further measurement dimensions may also be acquired [8], [9]. For high-dimensional data, it quickly becomes infeasible to sample the field uniformly, and recent development has aimed at instead using random sampling (see, e.g., [10]–[12]). For example, a recent study of 4-D NMR measurements that would have taken about 2.5 years to perform using regular sampling was shown to be possible to construct in merely 90 hours using a non-uniform sampling scheme [13]. This has also led to further studies aiming to optimize the selection of sampling point to achieve the best possible performance [14], [15].

To allow for a computationally efficient estimation of such signals, we here extend upon the sparse exponential mode analysis (SEMA) method introduced in [7], exploiting the recently developed concept of wideband dictionaries [16], [17] to accelerate the estimation of the frequencies of the modes. As wideband dictionaries allow for the use of an initially coarse grid, without risking to miss closely spaced signal component, the frequency regions of interest can be determined efficiently in an initial estimation, which are then iteratively refined to yield high-resolution estimates of the present frequency and damping components, without assuming a priori knowledge of the model order of the signal.

II. SIGNAL MODEL

Consider a D -dimensional signal consisting of K damped modes, such that an observation x_{τ} at a sampling point τ_n , where $\tau_n = [t_n^{(1)} \ t_n^{(2)} \ \dots \ t_n^{(D)}]^T$, with $t_n^{(d)}$ denoting the sampling time in dimension d , may be well modeled as

$$x_{\tau_n} = \sum_{k=1}^K g_k \prod_{d=1}^D \xi(f_k^{(d)}, \beta_k^{(d)})^{t_n^{(d)}} + \epsilon_{\tau_n}, \quad (1)$$

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where $\xi(f_k^{(d)}, \beta_k^{(d)}) = e^{2\pi i f_k^{(d)} - \beta_k^{(d)}}$, g_k denotes the complex amplitude of mode k , and ϵ_τ is an additive noise term, here assumed to be a white circularly symmetric Gaussian noise¹. Assuming that the signal is observed over N , in general non-uniformly spaced, multidimensional sampling points, let $\Omega = \{\tau_n, n = 1, 2, \dots, N\}$ denote the set of samples. The corresponding signal measurement vector, \mathbf{y} , may then be expressed as

$$\mathbf{y} = \sum_{k=1}^K g_k \tilde{\mathbf{a}}_k^\Omega + \boldsymbol{\epsilon}^\Omega, \quad (2)$$

where

$$\tilde{\mathbf{a}}_k^\Omega = \left[\prod_{d=1}^D \xi(f_k^{(d)}, \beta_k^{(d)}) t_1^{(d)} \quad \dots \quad \prod_{d=1}^D \xi(f_k^{(d)}, \beta_k^{(d)}) t_N^{(d)} \right]^T \quad (3)$$

$$\boldsymbol{\epsilon}^\Omega = \left[\epsilon_{\tau_1} \quad \dots \quad \epsilon_{\tau_N} \right]^T, \quad (4)$$

or, in matrix form, as

$$\mathbf{y} = \tilde{\mathbf{A}}^\Omega \mathbf{g} + \boldsymbol{\epsilon}^\Omega, \quad (5)$$

with

$$\tilde{\mathbf{A}}^\Omega = \left[\tilde{\mathbf{a}}_1^\Omega \quad \tilde{\mathbf{a}}_2^\Omega \quad \dots \quad \tilde{\mathbf{a}}_K^\Omega \right] \quad (6)$$

$$\mathbf{g} = \left[g_1 \quad g_2 \quad \dots \quad g_K \right]^T. \quad (7)$$

The problem of interest is thus to estimate the amplitudes, frequencies, and dampings of the K modes, without assuming knowledge of K .

III. THE WIDEBAND SEMA ESTIMATOR

As shown in [7], estimating the parameters detailing the K modes may be formed as the solution to

$$\underset{\mathbf{x}}{\text{minimize}} \quad \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_1, \quad (8)$$

where $\lambda > 0$ is a user-determined regularization parameter determining the sparsity of the solution, and \mathbf{A} denotes the dictionary matrix constructed over all considered parameter candidates, i.e., a column of \mathbf{A} details the evolution of a candidate component over the set of sampling points Ω . Clearly, the dimensionality of \mathbf{A} will grow rapidly with a growing number of modes, dimensions, and parameter candidates, making the minimization in (8) computationally cumbersome even for small problems. For high dimensional problems, or when a fine grid of parameters are required to avoid the risk of missing signal components, as is typically the case in spectroscopy, the minimisation quickly becomes infeasible.

To alleviate this problem, one may formulate efficient algorithms in the case of uniformly sampled data, exploiting the inherent structure in \mathbf{A} and that the resulting columns will be Fourier vectors [7]. As such a solution is not feasible for non-uniformly sampled data, we here proceed to formulate a solution exploiting wideband dictionary elements in order to reduce the dimensionality of the problem. Such dictionary elements are formed by integrating the contribution from all

¹In spectroscopy, this is an appropriate model as the additive noise primarily results from thermal (Johnson) noise.

Algorithm 1 The WSEMA algorithm

- 1: Select initial number of hypercubes P and construct hypercubes $\mathcal{H}_p, p = 1, \dots, P$.
 - 2: **repeat**
 - 3: Construct dictionary \mathbf{A} according to (12) from the hypercubes.
 - 4: Solve (8) using ADMM.
 - 5: Determine the set of active components $\mathcal{I} = \{p : |\mathbf{x}_p| > 0\}$.
 - 6: Construct new hypercubes subdividing $\mathcal{H}_p, p \in \mathcal{I}$ and discard hypercubes $\mathcal{H}_p, p \notin \mathcal{I}$.
 - 7: **until** Desired frequency resolution is attained
 - 8: Do NLS estimation of $\beta_k^{(d)}$ and $f_k^{(d)}, d = 1, \dots, D, k = 1, \dots, \hat{K}$, according to [7], where \hat{K} is the estimated number of modes.
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components between adjacent (narrowband) grid points. For example, in the one-dimensional case, for the non-damped case, this implies that a dictionary element should be formed by integrating the contribution from frequencies between to adjacent grid points, say f_a and f_b , such that [16], [17]

$$\begin{cases} 1, & \text{for } f_a \leq f \leq f_b \\ 0 & \end{cases} \xrightarrow{\mathcal{F}^{-1}} \frac{e^{2i\pi f_b t} - e^{2i\pi f_a t}}{2i\pi t}. \quad (9)$$

Such a dictionary element will thus cover the full band of frequencies, ensuring that any off-grid component is not missed, as would typically be the case for an ordinary (narrowband) dictionary (see, e.g., [18], [19]). By then reforming the dictionary for the activated candidates, one may efficiently zoom in on the regions of interest, refining these estimates. As shown in [16], [17], this allows one to use dictionaries substantially smaller than the number of measured samples, without the risk of missing components. This in turn allows for a dramatic reduction in the required computational complexity, especially for higher dimensional problems. Letting \mathcal{H}_p denote a D -dimensional hypercube in the frequency space, we define the wideband dictionary elements as

$$\mathbf{a}_p^\Omega = \left[\psi(\tau_1, \boldsymbol{\beta}_p, \mathcal{H}_p) \quad \dots \quad \psi(\tau_N, \boldsymbol{\beta}_p, \mathcal{H}_p) \right]^T, \quad (10)$$

where

$$\psi(\tau_n, \boldsymbol{\beta}, \mathcal{H}) = \int_{\mathcal{H}} \prod_{d=1}^D \xi(f^{(d)}, \beta^{(d)}) t_n^{(d)} df^{(1)} \dots df^{(D)}. \quad (11)$$

Each resulting wideband element is thus formed by integrating a damped sinusoid over the D -dimensional hypercube, for given values of the damping parameters $\beta^{(p)}$. The wideband SEMA (WSEMA) estimator is then formed as follows:

Initially, the frequency space $\mathcal{D} = [0, 1]^D$ is spanned by $\mathcal{H}_p, p = 1, \dots, P$, with $\cup_{p=1}^P \mathcal{H}_p = \mathcal{D}$ and $\mathcal{H}_p \cap \mathcal{H}_q = \emptyset$, for $p \neq q$. Here, as to promote computational speed, P is chosen to be a relatively small number². The corresponding dictionary

²As discussed in [17], P may typically be chosen as $N/3^D$ in order to achieve a good trade-off between computational complexity and required level of refinement steps

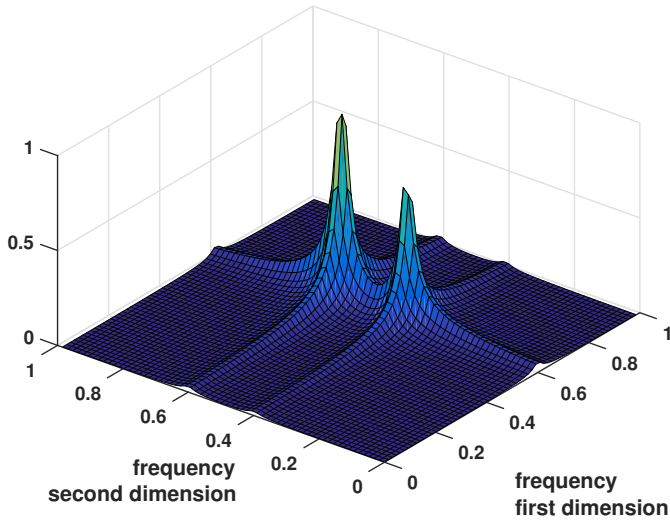


Fig. 1. Magnitude of the Fourier transform of a ground truth signal containing two modes.

\mathbf{A} is then formed as

$$\mathbf{A} = [\mathbf{a}_1^\Omega \quad \dots \quad \mathbf{a}_P^\Omega], \quad (12)$$

with, initially, the damping parameters β_p being set to zero. Starting from a set of initial frequency estimates obtained by solving (8) using this coarse frequency gridding, one may then iteratively increase the resolution of the estimates by sub-dividing the hypercubes \mathcal{H}_p corresponding to non-zero elements of the coefficient vector \mathbf{x} , while discarding the hypercubes corresponding to zero elements of \mathbf{x} . Thus, parts of the frequency space \mathcal{D} containing no power is sequentially disregarded, whereas sections of non-zero power are becoming more finely gridded. This zooming procedure may then be iterated until a desired frequency resolution is attained.

After forming frequency estimates using the above refinement procedure, the damping coefficients are then estimated using a non-linear least-square (NLS) step, as in [7]. This is done by minimizing the NLS cost function for each activated component over the corresponding frequency region and allowed range of damping coefficients, thus also further refining the frequency estimates. This yields an estimate of the damping components associated with each activated component, as well as a refined frequency estimate. To minimize the criterion in (8), one could, for example, use the alternating direction method of multipliers (ADMM) (see, e.g., [20]), which converges under quite mild assumptions on the objective function [21]. In this work, we use such an implementation, together with the so-called re-weighting framework as described in [22], as to increase the sparsity of the coefficient vector \mathbf{x} . The resulting WSEMA algorithm³ is summarized in Algorithm 1. It should here be noted that using an ADMM implementation, the most computationally expensive algorithm step requires $\mathcal{O}(P^3)$ operations, where

³An implementation of the resulting algorithm is available on the last author's webpage (upon acceptance).

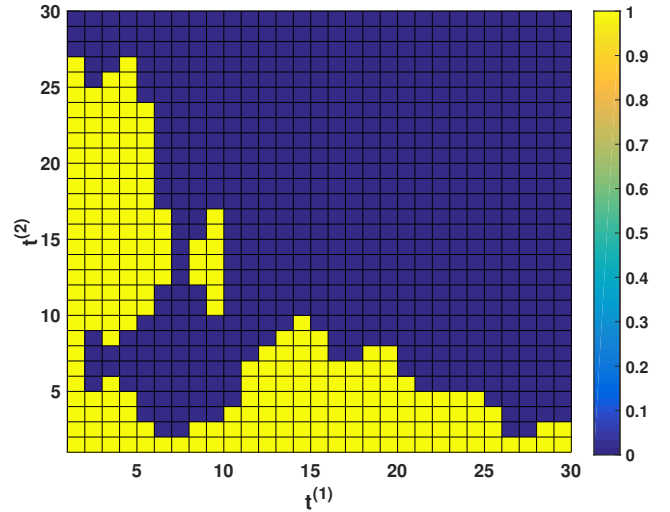


Fig. 2. Non-uniform sampling scheme. Here, the value 1 indicates that a sampling time has been selected.

P is the number of dictionary atoms. Thus, as representing a signal consisting of N samples in general requires at least $P = N$ narrowband dictionary atoms, and often more to achieve the desired resolution, the introduction of the proposed wideband scheme significantly decreases the computational complexity of the algorithm [16].

IV. NUMERICAL EXAMPLES

As an illustration of the proposed estimator WSEMA's applicability to non-uniformly sampled signals, consider a 2-D signal consisting of two damped sinusoids of magnitudes 1 and 0.7, with frequencies $f_1^{(1)} = 0.6$, $f_1^{(2)} = 0.6$, and $f_2^{(1)} = 0.6$, $f_2^{(2)} = 0.4$, respectively. Also, let $\beta_k^{(d)} = 0.1$ for $k = 1, 2$, $d = 1, 2$, and let the signal be contaminated by circularly symmetric white Gaussian noise of variance $\sigma^2 = 10^{-2}$. The magnitude of the 2-D Fourier transform of the ground truth signal is shown in Figure 1. As may be noted, its support is a set of non-zero measure due to the dampings. From a grid of dimension 30×30 with uniform sampling times, we select a total of 225 samples, i.e., 25% of the available samples, according to the method proposed in [14], [15], yielding a non-uniform set of samples. The sampling scheme is illustrated in Figure 2, where the value 1 indicates that a sampling time is selected. The Lomb-Scargle periodogram estimate of the non-uniformly sampled signal is displayed in Figure 3. As may be noted, the estimate contains a multitude of spurious peaks of power resulting from the non-uniform sampling pattern. The magnitude of the Fourier transform obtained by applying the WSEMA estimator to the same signal samples is shown in Figure 4. It should be noted that the WSEMA estimate accurately represents both the location and the shape of the modes, clearly illustrating the proposed methods applicability to non-uniformly sampled signals.

Continuing with examining the robustness of the proposed estimator, we consider its recovery rate for a multi-mode

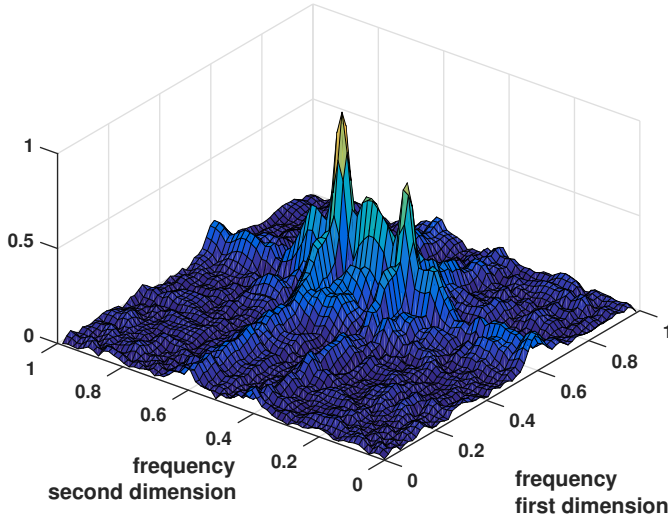


Fig. 3. The Lomb-Scargle periodogram estimate of the signal in Figure 1 when being measured at the sampling times shown in Figure 2.

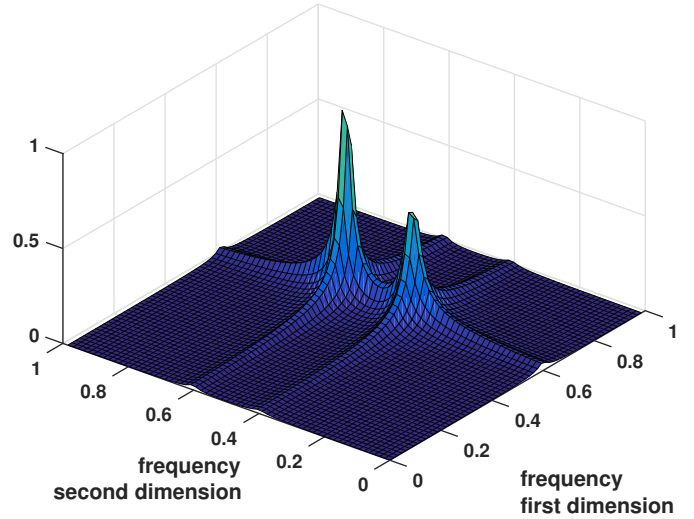


Fig. 4. The WSEMA estimate of the signal in Figure 1 when being measured at the sampling times shown in Figure 2.

signal. The simulated signal is formed of nine modes, and is uniformly sampled over each dimension, with frequencies randomly drawn on the interval $[1/N_d, 1-1/N_d]$, for each dimension, where N_d denotes the number of samples in dimension d . The frequencies are further restricted to be at least $1/N_d$ from any other frequency. Figure 5 illustrates the recovery rate for varying numbers of samples N_d , $d = 1, 2$, and initial number of hypercubes partitioning the 2-D frequency space, with recovery being defined as correctly identifying exactly nine modes, each estimated mode being less than $1/2N_d$ from the true frequency, for each dimension. The results are computed using 150 Monte Carlo-simulations, where each simulation is corrupted by an additive circularly symmetric Gaussian white noise. The signal-to-noise ratio (SNR) of the signals is $\text{SNR} = 15$ dB, where $\text{SNR} = 10 \log_{10}(\sigma_x^2/\sigma_e^2)$, with σ_x^2 being the variance of the signal and σ_e^2 being the variance of the noise. As can be seen from the figure, the proposed method quickly achieves full recovery as the number of samples and/or dictionary elements increases.

Further, to examine the statistical performance of WSEMA, in terms of accuracy of the parameter estimates, we consider a simulated 2-D signal, containing two damped modes, with unit magnitude and frequencies $f_1^{(1)} = 0.2$, $f_1^{(2)} = 0.6$, $f_2^{(1)} = 0.7$, and $f_2^{(2)} = 0.3$. To ensure that the frequencies are off-grid, each frequency is randomly perturbed by a uniform noise over the interval $[0, 0.04]$, for each Monte Carlo simulation. For each simulation, the damping parameters are randomly selected on the interval $[0.014, 0.022]$, for each mode and dimension, and the initial phases are randomly selected on the interval $[0, 2\pi)$. The signal is uniformly sampled on the 2-D interval $[0, \sqrt{N} - 1] \times [0, \sqrt{N} - 1]$, with a total of $N = 784$ samples.

Figure 6 shows the estimation performance of the WSEMA estimate as compared to the statistically efficient (parametric) subspace-based PUMA estimator [2], as well as the corre-

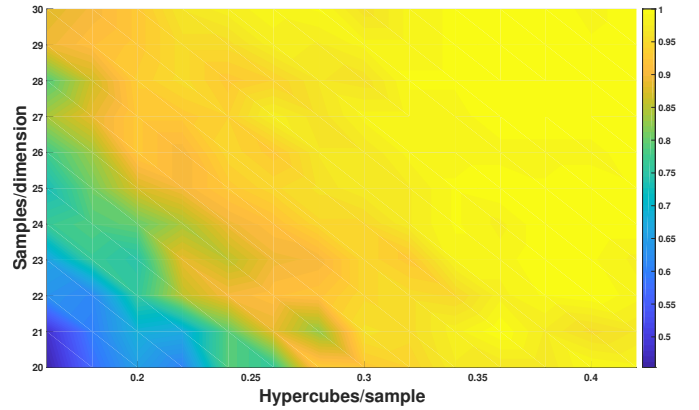


Fig. 5. Recovery rate for the proposed method for 2-D signals consisting of nine modes, for varying numbers of samples and dictionary atoms.

sponding average⁴ Cramér-Rao lower bound (CRLB) [23]. The signal is corrupted by an additive circularly symmetric Gaussian white noise of variance σ_e^2 ; the shown results are the root mean squared errors (RMSEs), defined as

$$\text{RMSE} = \sqrt{\frac{1}{MK} \sum_{m=1}^M \sum_{k=1}^K (\theta_{m,k} - \hat{\theta}_{m,k})^2}, \quad (13)$$

where K denotes the number of modes, M the number of Monte Carlo-simulations, whereas $\theta_{m,k}$ and $\hat{\theta}_{m,k}$ are the true and the estimated parameter value, respectively. The results are computed using $M = 1000$ Monte Carlo-simulations, for each noise power. As shown in the figure, the (semi-parametric) WSEMA estimator is able to achieve a performance similar to the parametric PUMA estimator, although only the latter is given oracle knowledge of the number of modes in the signal. To avoid outliers corrupting the results, simulations during

⁴The shown average CRLB is computed as the average of the CRLBs formed for the true parameters in each simulation.

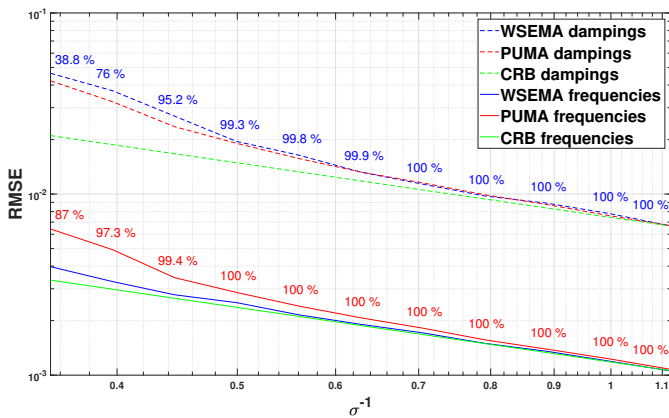


Fig. 6. The RMSE for WSEMA and PUMA as compared with the (average) root CRB for the summed frequencies and damping parameters. The number of samples used for each SNR is displayed in blue for WSEMA and in red for PUMA.

which an algorithm failed to recover the correct frequencies were removed. The number of retained samples for each algorithm and noise level are shown in Figure 6, indicating that WSEMA is able to recover the correct modes almost as often as PUMA for low SNRs, whereas both methods were found to recover the modes correctly for higher SNRs.

Finally, in order to illustrate the proposed frameworks applicability to measured data, we consider a 2-D NMR signal obtained from a ^{15}N -HSQC experiment made on a Histidine sample. Figure 7 shows the 2-D periodogram of the 50×50 uniformly sampled measurements of the signal. Superimposed are the estimates obtained by applying WSEMA to a random, non-uniform subset of size 40×40 of the available samples. As can be seen, the signal consists of a number of components of varying powers, all which may be reasonably well modeled as damped complex sinusoids. As seen in the figure, WSEMA is able to correctly identify these components despite having access to only 64% of the available samples.

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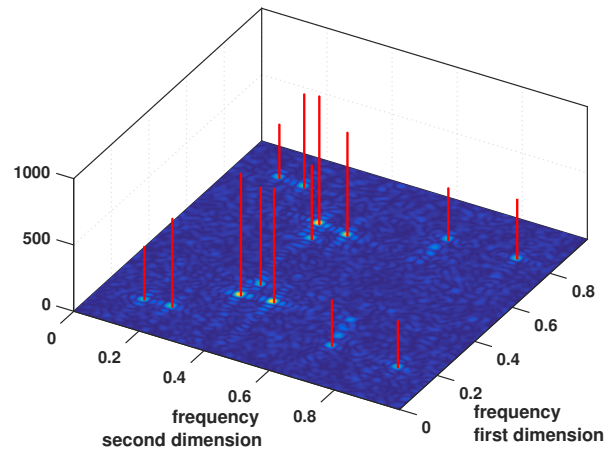


Fig. 7. Periodogram and WSEMA estimates of a measured 2-D NMR signal.