Computationally Efficient Estimation of Multi-Dimensional Spectral Lines

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COMPUTATIONALLY EFFICIENT ESTIMATION OF MULTI-DIMENSIONAL SPECTRAL LINES

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ABSTRACT

In this work, we propose a computationally efficient algorithm for estimating multi-dimensional spectral lines. The method treats the data tensor's dimensions separately, yielding the corresponding frequency estimates for each dimension. Then, in a second step, the estimates are ordered over dimensions, thus forming the resulting multidimensional parameter estimates. For high dimensional data, the proposed method offers statistically efficient estimates for moderate to high signal to noise ratios, at a computational cost substantially lower than typical non-parametric Fourier-transform based periodogram solutions, as well as to state-of-the-art parametric estimators.

Index Terms— High-dimensional data, Efficient algorithms, Spectral analysis, Parameter estimation, Sparse signal modeling.

1. INTRODUCTION

High dimensional data occurs in a variety of fields, the processing of which often requires computationally intensive analysis algorithms. In this work, we examine the problem of computationally efficient estimation of multidimensional sinusoidal data, such as occurring in, for instance, spectroscopic applications. Typically, for such problems, the high-resolution evaluation of the signal characteristics can require both notable computational efforts as well as vast memory requirements, and several efforts have been made to propose various forms of parametric and semi-parametric estimators (see, e.g., [1, 2]). In particular, the two-dimensional (2-D) case has been investigated in several works, such as [3–5], wherein the authors examine algorithms based on the problem's eigenvector structure, exploit a sparsity framework, as well as a subspace framework, respectively. Further works include [6], which examined the 3-D case, [7, 8], wherein different compressed sensing methods are compared for high dimensional NMR signals, and [8, 9], which examined high-dimensional subspace based estimators. Several works also focus on one of the computationally most efficient ways of forming multidimensional sinusoidal parameter estimates, namely the multi-dimensional periodogram, formed as the square of the absolute value of the Fast Fourier Transform (FFT) of the data [10]. Although computationally efficient, the method is well known to suffer from low resolution and/or high leakage [11]. However, when dealing with high-dimensional data sets, both the memory and the computational requirements quickly becomes cumbersome. In this work, we assume data with a relatively high signal-to-noise ratio (SNR) [12], such that each fiber of the data tensor contains notable information about the parameters. Exploiting this, we examine a non-parametric divide-and-conquer approach allowing for the forming of statistically efficient estimates, while requiring substantially less memory and computational complexity than corresponding FFT-based estimators. In order to do so, the proposed method first decouples a subset of fibers from the data tensor, in each dimension, and forms an initial estimate using these. These estimates are then ordered over dimensions, such that the estimates in each dimension are matched. Finally, the full data set is utilized to refine the initial estimate. Numerical examples illustrate the statistically efficient performance of the proposed estimator, as well as the required computational complexity as compared to both the multi-dimensional periodogram and the commonly used efficient parametric estimator FB-Root-MUSIC proposed in [9].

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2. PROBLEM STATEMENT

Let $\mathcal{Y}$ be an $N_1 \times \cdots \times N_M$ data tensor consisting of K multidimensional sinusoidals, where M denotes the number of dimensions and N_m the number of samples in dimension m, respectively. Furthermore, let $\mathcal{A}_{m,\boldsymbol{L}_m}(\mathcal{Y})$ denote the operator that extract the $\boldsymbol{L}_m$th fiber in mode-m from the tensor $\mathcal{Y}$ (see, e.g., [13] for a more detailed exposé of tensor notation), where

$$\boldsymbol{L}_m = \{\ell_1, \ldots, \ell_{M-1}\} \tag{1}$$

yielding a column vector fixing every index but one. As an example, consider the matrix $\mathbf{Y}$ defined as

$$\mathbf{Y} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \tag{2}$$

Algorithm 1 The DICO algorithm

Extract B fibers from each of the M dimensions.
for $m = 1, \dots, M$ **do**
  Compute the average periodogram using (7), and extract the dominating $\hat{K}_m$ frequencies.
end for
Create the dictionary $\mathbf{D}$ using (8)-(10), and solve (11).

Then, $\mathcal{A}_{1,2}(\mathbf{Y}) = [\ 2 \quad 5 \quad 8\ ]^T$, with $(\cdot)^T$ denoting the transpose, yielding the 2nd column along the first dimension. Similarly, $\mathcal{A}_{2,1}(\mathbf{Y}) = [\ 1 \quad 2 \quad 3\ ]^T$, yielding the first row in the second dimension. Let

$$\boldsymbol{\tau} = \left[\ t_{i_1}^{(1)} \quad t_{i_2}^{(2)} \quad \dots \quad t_{i_M}^{(M)}\ \right] \tag{3}$$

where $t_{i_m}^{(m)}$ denotes the i_mth (possibly non-uniform) sampling point in dimension m. Then, the observation at sample point $\boldsymbol{\tau}$ may be expressed as

$$y_{\boldsymbol{\tau}} = \sum_{k=1}^{K} \alpha_k \prod_{m=1}^{M} e^{2i\pi f_k^m t_{i_m}^{(m)}} + e_{\boldsymbol{\tau}} \tag{4}$$

where $e_{\boldsymbol{\tau}}$ denotes an additive noise term, here assumed to be an independent identically distributed zero-mean Gaussian distributed random variable, $f_k^{(m)}$ the normalized frequency for term k and dimension m, and where α_k denotes the complex amplitude of term k. It should be stressed that the number of sinusoidal components, K, is assumed to be unknown, and should thus be estimated along with the other model parameters.

The typical solution to this problem is to form the frequency estimates from the $\hat{K}$ dominant components in a multi-dimensional periodogram estimate, where $\hat{K}$ is an estimate of the number of components in the signal, usually estimated from the data using some simple cut-off rule or an information-theoretic setup [11, 14–16]. Such an operation requires $\mathcal{O}(\mathcal{P}_M log(\mathcal{P}_M))$ operations, where

$$\mathcal{P}_M = \prod_{\ell=1}^{M} P_\ell \tag{5}$$

with P_ℓ denoting the number of (zero-padded) frequencies over which the estimate should be evaluated over along dimension ℓ. Without loss of generality (w.l.g.), we will to simplify notation in the following assume that $P_\ell = P$, $\forall \ell$. For low dimensional data, such a solution is often computationally attractive, whereas for higher dimensions the complexity quickly grows to be intractable. Consider, for example, the 4-D case with $P = 512$, implying that $> 10^{11}$ operations are needed to form the estimate, as well as the allocation of a vast amount of memory. In this work, we consider high-dimensional data sets having moderate to high SNRs, such as those occurring, for instance, in NMR spectroscopy (see, e.g., [7]).

Algorithm 2 The DICO-NLS algorithm

Form the DICO residual, $\boldsymbol{r} = \mathbf{y} - \mathbf{D}\boldsymbol{x}$.
for $i = 1, \dots, I_{\text{max}}$ **do**
  for $k = 1, \dots, \hat{K}$ **do**
    Form $\tilde{\boldsymbol{r}}_k = \boldsymbol{r} + \mathbf{D}_k \boldsymbol{x}_k$
    for $m = 1, \dots, M$ **do**
      Keeping all dimensions but m fixed, form $\tilde{\mathbf{D}}_{k,m}$, and minimize (12) over $f_m^{(k)}$.
      Update $\tilde{\boldsymbol{r}}_k$ using the found estimate.
    end for
  end for
end for

3. DIVIDE AND CONQUER

Given that the data set is assumed to have a relatively high SNR, it can be noted that one ought to be able to form a reasonable initial estimate based on only a subset of the data. Using this notion, the proposed algorithm extracts a small set of B_ℓ fibers from the ℓth dimension of the data tensor, such that

$$\mathbf{y}_{k,\ell} \triangleq \mathcal{A}_{k,\boldsymbol{L}_\ell^{(\ell)}}(\mathcal{Y}) \in \mathcal{C}^{N_\ell \times 1} \tag{6}$$

for $k = 1, \dots, B_\ell$ and $\ell = 1, \dots, M$. W.l.g., we will in the following assume that $B_\ell = B$, $\forall \ell$. From this set of BM vectors, we form initial estimates of all frequencies, in each of the dimensions. This may be done in a variety of ways; here, in the interest of computational simplicity, we form the estimates along each dimension using an averaged periodogram, such that

$$\hat{\boldsymbol{\phi}}_m = \sum_{b=1}^{B} \frac{1}{BN_m} \left| \sum_{t=1}^{N_m} y_{m,b}(t) e^{-i2\pi t \frac{p}{P}} \right|^2 \tag{7}$$

for all considered frequencies $p = 1, \dots, P$. An estimate of the number of active components can then be formed using either some simple cut-off rule, or more sophisticated model order estimation techniques, such as, for instance, those presented in [11, 15, 16]. Clearly, instead of (7), an alternative estimate may be formed using, e.g., Capon- or LASSO-based estimators [], or via parametric estimators such as MUSIC and ESPRIT, although the latter necessitating also a model order estimation as a part of the estimation process.

After forming such an initial estimate of the $\hat{K}_\ell$ frequencies, in dimension ℓ, $\forall \ell$, the resulting estimates in each dimension must be grouped over dimensions, such that the appropriate frequencies in each dimension are matched with each other. Since the number of possible pairings increases exponentially with the number of found frequencies in each dimension, we propose to perform the pairing using sparse

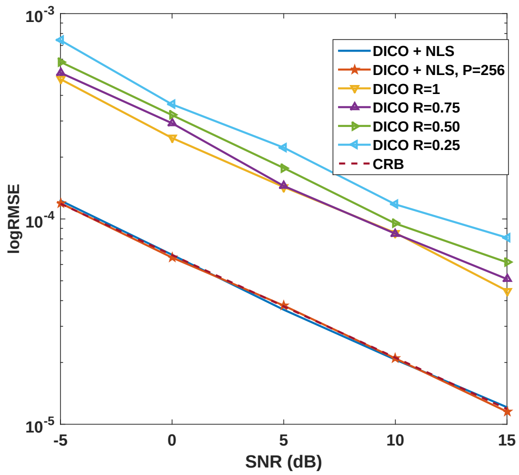

Fig. 1. The log RMSE for DICO and DICO-NLS for different settings, as compared to the CRB.

modeling [17]. To do so, let

$$\mathbf{D}_m = \left[\begin{array}{ccc} \boldsymbol{d}_1^{(m)} & \dots & \boldsymbol{d}_{K_m}^{(m)} \end{array} \right] \tag{8}$$

$$\boldsymbol{d}_k^{(m)} = \left[\begin{array}{cccc} 1 & e^{2i\pi f_k^{(m)}} & \dots & e^{2i\pi f_k^{(m)}(N_m-1)} \end{array} \right]^T \tag{9}$$

for $m = 1, \dots, M$, denote M sub-dictionaries over the found frequencies, in their respective dimensions (we note that a similar dictionary was introduced in 2-D case in [18]). Combining the dictionary as

$$\mathbf{D} = \mathbf{D}_M \otimes \cdots \otimes \mathbf{D}_1 \tag{10}$$

where $\otimes$ denotes the Kronecker product, the frequencies may be matched by solving

$$\underset{\boldsymbol{x}}{\text{minimize}} \quad \frac{1}{2} \left|\left|\text{vec}\left(\mathcal{Y}\right) - \mathbf{D}\boldsymbol{x}\right|\right|_2^2 + \lambda \left|\left|\boldsymbol{x}\right|\right|_1 \tag{11}$$

where vec$(\cdot)$ is the vectorization operator, stacking the tensor to a vector corresponding to the structure in $\mathbf{D}\boldsymbol{x}$. As shown in [19], the minimization in (11) may be formed efficiently using an Alternating Direction Method of Multipliers (ADMM) implementation. Algorithm 1 summarizes the resulting DIvide and COnquer (DICO) algorithm. It should be noted that (11) could theoretically be solved directly for all considered frequency grid points, without the initial selection step outlined above, although such a solution would be practically infeasible due the resulting $(N_1 \cdots N_M \times P^M)$-dimensional dictionary. Given the resulting frequency ordering, the initial estimates may be refined using a simple non-linear least squares (NLS) technique, using either gradient steps or a grid search, as summarized in Algorithm 2, i.e., such that the kth frequency in the mth dimension is estimated as

$$\underset{f_m^{(k)}}{\text{minimize}} \quad \tilde{\boldsymbol{r}}_k^H \mathbf{\Pi}_{\tilde{\mathbf{D}}_{k,m}}^{\perp} \tilde{\boldsymbol{r}}_k \tag{12}$$

with $\tilde{\boldsymbol{r}}_k$ denoting the residual formed by extracting all but the kth component from $y_{\boldsymbol{\tau}}$, $\tilde{\mathbf{D}}_{k,m}$ the corresponding dictionary, and

$$\mathbf{\Pi}_{\tilde{\mathbf{D}}_{k,m}}^{\perp} = \mathbf{I} - \tilde{\mathbf{D}}_{k,m} \left(\tilde{\mathbf{D}}_{k,m}^H \tilde{\mathbf{D}}_{k,m} \right)^{-1} \tilde{\mathbf{D}}_{k,m}^H \tag{13}$$

the projection onto the space orthogonal to the one spanned by the dictionary. Assuming, w.l.g., $N_\ell = N$, $\forall \ell$, samples in each dimension, the DICO algorithm requires about $MRPN^{M-1} \log(P)$ operations for the initial step, where $R = BN^{1-M}$ denotes the proportion of data used to form the initial estimate. The averaging in (7) requires $MRNP^{M-1}$ operations, and the extraction of the peaks amounts to $3MP$ further operations, followed by roughly $3MN^{M+1}$ operations for the ADMM implementation, if implemented utilizing the Kronecker structure (see also [20] and [21]). Finally, the NLS using a grid search requires about $3QM\hat{K}N_{\text{tot}}$ operations, where Q and $\hat{K}$ denote the number of NLS evaluations along dimension m and the number of found M-dimensional sinusoids, respectively.

4. NUMERICAL EXAMPLES

In this section, we evaluate the performance and complexity of the proposed method using simulated multidimensional sinusoidal data. As an example, we consider a uniformly sampled 3-D data tensor of size $40 \times 40 \times 40$, containing $K = 3$ 3-D sinusoids, with frequency modes

$$\boldsymbol{f}_1 = \frac{\pi}{3} [\ 0.3 \quad 0.2 \quad 0.1\ ] \tag{14}$$

$$\boldsymbol{f}_2 = \frac{\pi}{3} [\ 0.6 \quad 0.4 \quad 0.5\ ] \tag{15}$$

$$\boldsymbol{f}_3 = \frac{\pi}{3} [\ 0.7 \quad 0.8 \quad 0.9\ ] \tag{16}$$

with unit magnitude and phase uniformly drawn from $[-\pi, \pi]$. Figure 1 shows the log root mean squared error (logRMSE) of the proposed estimator for different settings (summed over all frequencies), as compared with the corresponding Cramér-Rao lower Bound (CRB), as derived in [22], as a function of the SNR, here defined as

$$\text{SNR} = 10 \log_{10} \left(\sigma^{-2} P_{\mathbf{y}} \right) \tag{17}$$

where $P_{\mathbf{y}}$ denotes the power of the signal and σ^2 the variance of the noise, respectively. The results have been computed using 100 Monte-Carlo simulations.

As seen in the figure, the DICO algorithm offers a good initial estimate, even if only using a low proportion of the available data. Adding the refinement step, it is clear that the DICO-NLS combination offers statistically efficient estimates. Here, all the estimators but one have been evaluated using a zero-padding of $P = 65536$ grid points, although as shown in the figure, the remaining, the combined DICO-NLS method will be efficient even using as little zero-padding

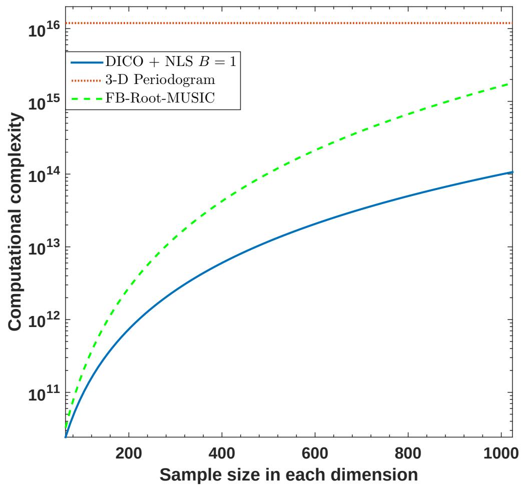

Fig. 2. The computational complexity of the 3-D periodogram, DICO-NLS, and the FB-Root-MUSIC algorithm, as a function of the data size, for 20 spectral lines.

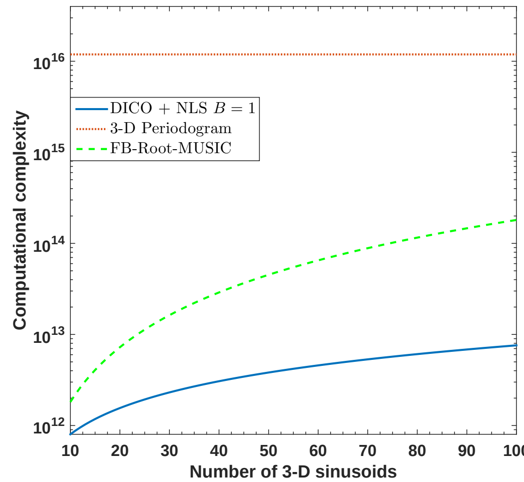

Fig. 3. The computational complexity of the 3-D periodogram, DICO-NLS, and the FB-Root-MUSIC algorithm, as a function of the number of spectral lines, for $N = 256$.

as $P = 256$. The maximum outer-loops in the NLS step, $I_{\max}$, was set to 3, where in each iteration the search area was narrowed down by a factor 100, which was evaluated over $Q = 100$ grid points. In order to select the number of frequencies in each dimension, we here, for simplicity, use a simple cut-off rule, such that all peaks larger than the average of the maximal and minimal value of (7) are treated as separate frequencies. Clearly, one may instead use more sophisticated model-order estimation techniques, such as AIC or BIC (see, e.g., [11, 14]). To avoid cluttering the figure, the FFT-based periodogram estimates are not shown as it is well known that these will also yield statistically efficient estimates for this setting, if using a sufficiently large zero-padding; here, in order to do so, it would require a total grid size of at least 2^{48}, for the 3-D FFT at SNR$= 10$. Similarly, it is well-known that several parametric estimators, such as the FB-Root-MUSIC algorithm presented in [9], will also achieve the CRB, if given full knowledge of the model order.

Next, we examine the computational complexity of the proposed DICO algorithm, as compared to the 3-D periodogram and the FB-Root-MUSIC algorithm. To do so, we mimic the 3-D NMR experiments detailed in [2, 7, 23], such that N varies from 64 to 1024, each containing 20 sinusoids. For DICO, we use $P = 4096$ and $I_{\max} = 5$, and the search area for the NLS narrowed down by a factor 100 for each iteration, using $Q = 100$ grid points in the NLS search. Figures 2-3 show complexity for DICO, the 3-D periodogram, and the FB-Root-MUSIC algorithm as a function of the data size and the number of sinusoids, respectively. Here, both the periodogram and the FB-Root-MUSIC algorithm have been allowed oracle model order information, whereas DICO estimates the number of frequencies using the above noted simple cut-off rule. Here, the periodogram uses a zero padding of $P = 65536$ grid points in each dimension, independently of the data size. It should be noted that such a small grid is not sufficient for its estimate to be even close to the CRB for large N. As is clear from the figures, the DICO-NLS estimate offers a statistically efficient estimate at a computational cost substantially lower than both the 3-D periodogram and the FB-Root-MUSIC algorithm. Furthermore, it should be noted that the DICO estimate does not require even a fraction of the memory requirements of the 3-D periodogram, as only the averaged estimate of the fibers in (7) need to be stored in memory. Finally, as is clear from the presentation above, the computational gain as compared to the periodogram and the FB-Root-MUSIC algorithm will grow even faster for higher dimensions.

5. CONCLUSIONS

In this work, we have presented a computationally and statistically efficient multi-dimensional sinusoidal frequency estimator. The proposed estimator exploits that notable information about the unknown frequencies may be found in a subset of the data tensor. This subset is used to form a first estimate that is then refined using the entire data set, estimating the number of spectral lines as a part of the procedure.

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