

Evaluation of Resolution Improvement Ability of a DSP Technique for Filter-Array-Based Spectrometers

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ABSTRACT

In this paper, we aim to evaluate the performance of the digital signal processing (DSP) algorithm used in [8] in order to improve the resolution of spectrometers with fixed number of low-cost, non-ideal filters. In such spectrometers, the resolution is limited by the number of filters. We aim to demonstrate via new experiments that the resolution improvement by six times over the conventional limit is possible by using the DSP algorithm as claimed by [8].

I. Introduction

Miniature spectrometers are key instruments that are required in various academic and industrial applications such as bio-medical, chemical, and environmental engineering^[1]. These spectrometers, built with integrated-filter arrays, provide superior portability, flexibility, and cost-effectiveness^[2,3]. The spectrometers also provide fine details about the various spectral components of the incident light. These spectral components reveal a wealth of information concerning the composition and the structure of the various objects being observed^[3]. The ability of a spectrometer to reveal fine information is usually attributed to its resolution. In recent years, researchers focus on improving the resolution of the filter-array based spectrometers^[4]. The resolution of these spectrometers depends on the number of filters and the transmittance characteristics of the filters. The filters with non-ideal characteristics cause severe distortion of

the raw signal spectrum obtained from the spectrometer. Therefore, it is difficult to resolve the distinct spectral components from the raw spectrum. To alleviate this problem, digital signal processing (DSP) techniques which process the raw signal spectrum are shown to be helpful. The current literature^[5-7] provides a few DSP techniques to reconstruct the original spectrum but not on improving the resolution of the spectrometer. Recently, the authors in [8] used a new DSP algorithm developed in [9] for improving the resolution of the spectrometers. The authors in [9] designed the algorithm using L_1 norm minimization which exploits the prior information that a signal is sparse and non-negative. Since light spectrum is non-negative, the authors in [8] tailored the algorithm in [9] in order to improve the resolution of miniature spectrometers. They show via synthetic spectrum data sets that the resolution can be improved six times beyond the conventional limit. However, the use of the algorithm for real world

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data sets are largely unknown.

In this paper, we evaluate the performance of the algorithm in [8]. In particular, we show how to employ the algorithm in [8] to more practical spectrum data sets. With a spectrum data set close to that of a metal halide arc lamp, we illustrate how the algorithm improves the resolution by six times. We begin this paper with a review of the data model, the algorithm and the measure of resolution of a spectrometer. We then provide our experiments results.

II. System Description

The raw spectrum y obtained from the spectrometer can be modeled as a system of linear equations as [8]

$$y = DAs + w, \quad s \geq 0 \quad (1)$$

where D is an $M \times N$ filter transmittance matrix with $M < N$ and A is an $N \times N$ Gaussian kernel matrix^[4] and s is a K -sparse spectrum (or signal), i.e., only K components of s are non-zero and the remaining components are zero and w is a noise vector. The original signal spectrum, x , admits a sparse representation^[4,8] in the kernel matrix A as

$$x = As \quad (2)$$

Let W denote the wavelength range of the signal spectrum x . Let Δ denote the spacing between the samples of x as well as s . We note that the dimension of y is $M \times 1$ and of s is $N \times 1$. Our goal is to obtain an estimate s_e of s from y (in Eq. (1)). Note that the dimension of y is much smaller than the dimension of the sparse signal s . Also, with $M < N$, the noiseless system in Eq. (1) is clearly underdetermined. In order to solve the underdetermined system, the authors in [8] used a new L1 norm minimization algorithm^[9] and thereby obtained an estimate s_e . The original signal spectrum can then be estimated as $x_e = As_e$. The accuracy of the spectrum estimation is measured by the mean square error (MSE):

$$MSE = \frac{1}{N} \| x - x_e \|^2 \quad (3)$$

III. Resolution of a Spectrometer

Traditionally, resolution of a spectrometer represents its ability to distinguish the peaks of two closely spaced spectral components of the input signal spectrum. The spectrometers that identify the closely spaced spectral components reveal fine details about the input signal spectrum. Thus, the quality of the spectrometers is usually specified in terms of how well the spectrometer resolves two closely spaced spectral components, which is perhaps good for the conventional spectrometers but not appropriate for a DSP based spectrometer. Therefore, the authors in [8] introduced a new way of measuring the resolution of a filter-array based spectrometer which uses a DSP algorithm. We briefly review their measure in this following paragraphs.

At a given spacing, $R_N = W/N$ ^[8] defines the maximum achievable resolution of the spectrometer as $R_{max} = u_N R_N$, where u_N is calculated by

$$u_N := \min_{u \in 1, 2, \dots, N-1} u \quad \text{subject to } MSE \leq \delta \quad (4)$$

where $\delta > 0$ is a user-defined MSE. Any two spectral components which are u apart from each other are resolvable if the MSE between the recovered (estimated) and the input signal spectrum is less than or equal to δ . Since the spacing is $R_N = W/N$, for a fixed W , increasing N decreases the spacing Δ . We increase N starting from M , since M is called resolution limit of the filter-array based spectrometers^[4]. When we increase N beyond M , the system in Eq. (1) becomes underdetermined (in the noiseless case). An underdetermined system which is solved by considering classical L_2 norm minimization does not offer a sparse solution [10].

Alternatively, the authors in [8], aim to solve the underdetermined system using L_1 norm minimization

techniques^[9]. To aid the L_1 norm minimization, they exploited the prior information that a signal spectrum is sparse as well as the values of the signal spectrum are non-negative. We provide a brief derivation steps of the algorithm in the next section.

IV. Non-Negative L_1 minimization (NNLM) Algorithm

We recall that we are given with only $M (<N)$ number of samples of the raw spectrum. We need to estimate N number of unknowns from M known values. The best, brute-force approach for recovering \mathbf{s} is to search for the sparsest vector \mathbf{s} which is consistent with \mathbf{y} . This leads to solving L_0 norm minimization problem which is known to be computationally intractable [9]. Interestingly, L_1 norm minimization provides a tractable solution to the problem in Eq. (1). The L_1 norm minimization problem for sparse signal recovery is given by [8]

$$\min_{\mathbf{s}} \|\mathbf{s}\|_1 + \frac{\tau}{2} \|\mathbf{y} - \mathbf{DAs}\|_2^2 \quad (5)$$

where τ is a non-negative parameter. We assign $\mathbf{B} = \mathbf{DA}$ and solve Eq. (5) as a linear programming problem with a non-negative spectrum constraint, \mathbf{s} greater than or equal to 0, as

$$\min_{\mathbf{s}} \mathbf{1}^T \mathbf{s} \text{ s.t. } \|\mathbf{Bs} - \mathbf{y}\|_2^2 \leq \epsilon, \mathbf{s} \geq 0 \quad (6)$$

The authors in [9] adopted the modern interior point method called primal-dual approach in order to solve the above linear programming problem and thereby found the optimal signal spectrum estimate \mathbf{s}_e . The authors in [8] adopted the algorithm from [9] and tailored it for spectrometers. The pseudo-code of their proposed algorithm in Table 1.

V. Results and Discussions

In this section, we aim to demonstrate the performance of the NNLM algorithm discussed in Section IV for various data sets. We first consider

a synthetic data with two spectral component to calculate the resolution as discussed in Section III. We then evaluate the performance of the algorithm for a spectral data similar to that of a metal halide arc lamp^[11]. We consider a spectrometer with $W = 800$ nm and $M = 40$ filter elements in the filter array^[12]. We first consider the signal length $N = 240$. The value of δ required in Eq. (4) is set as $1e-3$. The original signal spectrum has a sparsity of $K = 2$. We choose two consecutive spectral components, as resolution is an issue to see if two closely spaced spectral components can be resolved or not.

Table 1. Pseudo code to solve Eq. (6) by Non-Negative L_1 minimization Method

Step 1	<p>Initialization: Choose $\gamma \in (0,1)$ and $\tau > 0$. Set the iteration index $l=0$, slack variable vector $\mathbf{v}^l = \mathbf{1}$ and the initial solution is set as $\mathbf{s}_\tau^l = \mathbf{1}$</p>
Step 2	<p>Computation of direction vectors: Let us define correlation vector $\mathbf{c} = \mathbf{B}^T(\mathbf{y} - \mathbf{Bs}_\tau^l)$. Let $\mathbf{S} = \text{diag}(s_1^l \cdots s_N^l)$, $\mathbf{V} = \text{diag}(v_1^l \cdots v_N^l)$, $\mathbf{1}^T = [1 \cdots 1] \in R^N$. Then the direction vectors $\Delta \mathbf{s}_\tau^l$ and $\Delta \mathbf{v}_\tau^l$ are obtained by using $\Delta \mathbf{s}_\tau^l = [\mathbf{V} + \tau \mathbf{SB}^T \mathbf{B}]^{-1} [\tau \mathbf{S} \mathbf{c} + \mathbf{S} \mathbf{v}^l - \mathbf{s}_\tau^l - \mathbf{S} \mathbf{V} \mathbf{1}]$ and $\Delta \mathbf{v}_\tau^l = \tau (\mathbf{B}^T \mathbf{B} \Delta \mathbf{s}_\tau^l - \mathbf{c}) - \mathbf{v}^l + \mathbf{1}$</p>
Step 3	<p>Step-size selection: Let α_0 be sufficient large positive number. Choose α^l to be the first number in the sequence $\alpha_0, \alpha_0 \gamma, \alpha_0 \gamma^2, \dots$ such that $\mathbf{v}^l + \alpha^l \Delta \mathbf{v}_\tau^l \geq \mathbf{0}$ and $\ F_\tau(\mathbf{s}_\tau^l, \mathbf{v}^l)\ _2 > \ F_\tau(\mathbf{s}_\tau^l + \alpha^l \Delta \mathbf{s}_\tau^l, \mathbf{v}^l + \alpha^l \Delta \mathbf{v}_\tau^l)\ _2$, where the matrix F_τ is obtained from the KKT condition^[4].</p>
Step 4	<p>Update: $\mathbf{s}_\tau^{l+1} = \mathbf{s}_\tau^l + \alpha^l \Delta \mathbf{s}_\tau^l$ and $\mathbf{v}^{l+1} = \mathbf{v}^l + \alpha^l \Delta \mathbf{v}_\tau^l$</p>
Step 5	<p>If $\ \mathbf{s}_\tau^l - \mathbf{s}_\tau^{l+1}\ \leq \epsilon$, then terminate with the estimate $\mathbf{s}_e = \mathbf{s}_\tau^{l+1}$. Find $\mathbf{x}_e = \mathbf{As}_e$. Otherwise, $l = l + 1, \tau = \beta \tau$ where $\beta > 1$ and go to Step 2.</p>

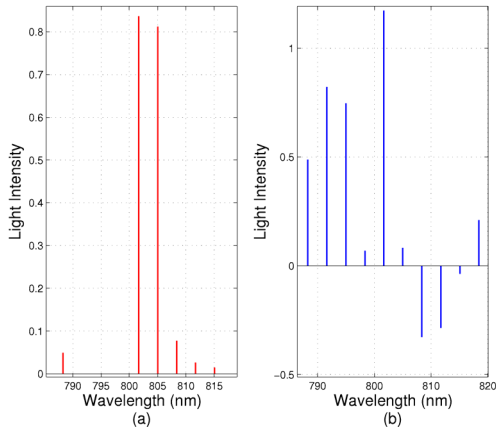


Fig. 1. Estimated signal spectrum in the sparse domain (a) using proposed NNLM algorithm (b) using L_2 technique

Fig. (1) shows the estimated signal spectrum in the sparse domain using the proposed and the L_2 based least square algorithm^[6]. The original signal spectrum contains two dominant spectral components located at 801.7 nm and 805 nm respectively. It is evident from Fig. 1(a) that the dominant spectral components are clearly resolved by the proposed algorithm. The additional spectral components that appear nearby the dominant spectral components are smaller in amplitude and do not affect the resolvability of the dominant spectral components. Since the two spectral components that are R_N apart from each other are distinctly resolved with the value of $u = 1$, the maximum spectral resolution obtained by using $N = 240$ is $R_{max} = 3.33$ nm (800 nm / 240) which is six times better than the conventional limit of $R_M = 20$ nm (800 nm / 40), assuming $u_M=1$. When we increase N further, we found that we cannot satisfy the user specified δ of $1e-3$. Thus, we stop at $N = 240$. We show in Fig. 1(b) the sparse spectrum estimated by using the conventional L_2 technique. It is evident from Fig. 1(b) that L_2 -based technique provides a non-sparse spectrum. Besides, the technique cannot resolve the two closely spaced spectral components.

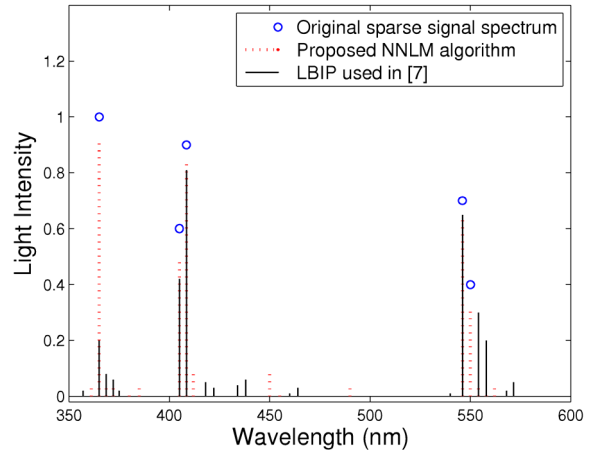


Fig. 2. Reconstruction of sparse signal spectrum by various L_1 algorithms

We now show that a resolution of 3.33 nm (as computed in the last paragraph) is achievable by using NNLM and also we illustrate the superior performance of the proposed NNLM over the log-barrier interior point (LBIP) algorithm in [7]. We consider a signal spectrum with 5 spectral components which resembles that of a metal halide arc lamp^[11] with spectral components located at 365 nm, 405 nm, 408.5 nm, 546 nm, and 550 nm, respectively. We note that the least separation among these spectral lines is 3.5 nm which is between the pair 405 nm and 408.5 nm. We aim to resolve these components. Figure 2 shows the original and the estimate of the sparse spectrum using the proposed NNLM and the LBIP. We note from Fig. 2 that NNLM correctly estimates the 5 wavelength components. In addition, NNLM clearly resolves the two closely spaced spectral components at 405 nm and 408.5 nm. This evidence supports the fact that NNLM is capable of resolving any two spectral components which are more than 3.33 nm apart. On the contrary, the estimate by the LBIP misses out the 550 nm wavelength component as shown in Fig. 2. Both, the NNLM and the LBIP, make some detection errors because of the presence of observation noise; but the errors made by NNLM are less significant than those by the LBIP. Based on these results and observations, we conclude that the accuracy of the proposed algorithm is better than the LBIP algorithm.

VI. Conclusions

In this paper, we discussed how to apply the algorithm used in [8] to more practical spectrum data sets. In particular, we considered a data set that resembles that of a metal halide arc lamp. We illustrated that the algorithm is able to resolve the spectral components that are more than 3.33 nm apart. With the same data set, we also demonstrated the superiority of the algorithm with that of the existing ones.

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