A New Signal Processing Technique for Improving Resolution of Spectrometers

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Abstract

In this paper, we present a signal processing approach to improve the resolution of a spectrometer with a fixed number of low-cost, non-ideal filters. We aim to show that the resolution can be improved beyond the limit set by the number of filters by exploiting the sparse nature of a signal spectrum. We obtained 6 times resolution improvement by modeling the signal spectrum as an underdetermined system of linear equations and solving it by designing a new non-negative L_1 norm minimization algorithm.

Ⅰ. Introduction

Spectrometers are highly demanded in various industrial and domestic applications [1]. Modern miniature spectrometers are filter array based and are fabricated using CMOS or Nano technology to bring down the size and cost. In recent years, researchers focus on improving the resolution of filter array based because the non-ideal filters in the spectrometer causes 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 [2] provides a few DSP techniques to reconstruct the original spectrum but not on improving the resolution of the spectrometer.

In this paper, we develop a new framework that determines an achievable resolution of a spectrometer. We aim to show that the achievable resolution of a spectrometer can be improved 6 times beyond the limit set by the number of filters, which was originally discussed in [3]. We show that an L_1 norm minimization based approach is more suitable than a classical L_2 norm minimization for solving an underdetermined system of linear equations. We design a new spectrum estimation algorithm using L_1 norm minimization that exploits the prior information that the signal spectrum is sparse and non-negative.

Ⅱ. System description

We model the raw spectrum $\boldsymbol{y}$ obtained from the spectrometer as a system of linear equations:

$$\boldsymbol{y} = D\Psi\boldsymbol{s} + \boldsymbol{w} \quad \boldsymbol{s} \geq 0 \tag{1}$$

where D is an $M \times N$ filter transmittance matrix with $M < N$ and Ψ is an $N \times N$ Gaussian Kernel and $\boldsymbol{s}$ is a K-sparse signal, i.e., only K components of $\boldsymbol{s}$ are non-zero and the remaining components are zero and $\boldsymbol{w}$ is the noise vector. The original signal spectrum is $\boldsymbol{x} = \Psi\boldsymbol{s}$. Let W_λ denote the total bandwidth of the signal $\boldsymbol{x}$. Let $\Delta\lambda_N = \frac{W_\lambda}{N}$ denote the spacing between the samples of $\boldsymbol{x}$ as well as $\boldsymbol{s}$. We note that the dimension of $\boldsymbol{y}$ is $M \times 1$ and of $\boldsymbol{s}$ is $N \times 1$. Our goal is to obtain an estimate $\hat{\boldsymbol{s}}$ of $\boldsymbol{s}$ from $\boldsymbol{y}$ given by Eq. (1). Note that the dimension of $\boldsymbol{y}$ is much smaller than the dimension of the sparse signal $\boldsymbol{s}$ and the noiseless system in Eq. (1) is clearly underdetermined. We design a new L_1 norm minimization algorithm for recovering the sparse spectrum $\boldsymbol{s}$ from the raw spectrum $\boldsymbol{y}$. The original signal spectrum can then be estimated as $\hat{\boldsymbol{x}} = \Psi\hat{s}$. The spectrum estimation accuracy is measured by the mean square error (MSE): $\mathrm{MSE} = \frac{1}{N}\|x - \hat{x}\|^2$.

Ⅲ. Resolution of a spectrometer

Traditionally, resolution of a spectrometer is 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 this resolution which perhaps good enough for the conventional spectrometers but not appropriate for those which utilize a DSP algorithm. In this section, therefore, we introduce a new way of measuring the resolution of a DSP based filter-array spectrometer.

At a given spacing $\Delta\lambda_N = \frac{W_\lambda}{N}$, we define the maximum achievable resolution of a spectrometer as $\Delta\lambda_{\max} = \mu_N \Delta\lambda_N = \mu_N \frac{W_\lambda}{N}$, where μ_N is given by

$$\mu_N := \min_{\mu \in \{1,2,\cdots,N-1\}} \mu \quad \text{subject to} \quad \mathrm{MSE} \leq \delta \tag{2}$$

where $\delta > 0$ is a user-defined MSE. We say that any two spectral components which are $\mu_N \Delta\lambda_N$ apart from each other are resolvable if the MSE between the recovered and the input signal spectrum is less than or equal to δ. Since the spacing between the samples is given by $\Delta\lambda_N = \frac{W_\lambda}{N}$, for a fixed W_λ, increasing N decreases the spacing $\Delta\lambda_N$. We increase N staring from M. When we increase N beyond M, the system Eq. (1) becomes underdetermined (in the noiseless

case). An underdetermined system which is solved by considering classical L_2 norm minimization does not improve the spectral resolution as shown in [4].

Alternatively, we aim to solve the underdetermined system using L_1 norm minimization techniques. To aid the L_1 norm minimization, we exploit the prior information that a natural signal spectrum sparse as well the values of the signal spectrum are non-negative. We provide a brief sketch of our new algorithm in the next section.

Ⅳ. Proposed non-negative L_1 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 $\boldsymbol{s}$ is to search for the sparsest vector $\boldsymbol{s}$ which is consistent with $\boldsymbol{y}$. This leads to solving L_0 norm minimization problem which is known to be computationally intractable. Interestingly, L_1 norm minimization provides a tractable solution to the problem in Eq. (1). Our L_1 norm minimization for sparse signal recovery is given by

$$\min_{\boldsymbol{s}} \|\boldsymbol{s}\|_1 + \tfrac{\tau}{2}\|\boldsymbol{y} - D\Psi\boldsymbol{s}\|_2^2 \qquad (3)$$

where τ is a non-negative parameter. We solve Eq. (3) as a linear programming problem with nonnegative spectrum constraint $\boldsymbol{s} \geq \boldsymbol{0}$ as

$$\min_{\boldsymbol{s}} \boldsymbol{I}^T\boldsymbol{s} \quad \text{s.t} \quad \|D\psi\boldsymbol{s} - \boldsymbol{y}\|_2^2 \leq \varepsilon,\ \boldsymbol{s} \geq \boldsymbol{0} \qquad (4)$$

In this paper, we have adopted the modern interior point method called primal-dual approach [3] that solves the above linear programming problem in order to find the optimal signal spectrum estimate $\hat{\boldsymbol{s}}$. In the next section we show the estimated spectrum using our proposed and the conventional methods [2].

Ⅴ. Results and Conclusions

In this section, we aim to demonstrate the performance of the proposed algorithm in Section Ⅳ. We consider a filter array with $M = 40$ elements. The W_λ of the spectrometer is 800nm. We first consider the filter length $N = 240$. The value of δ required in Eq. (2) 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 close spectral components can be resolved or not.

Figure (1) shows the estimated signal spectrum in the sparse domain using the proposed and the conventional algorithm in [2]. The original signal spectrum contains two dominant spectral components located at 828.46nm and 831.8nm respectively.

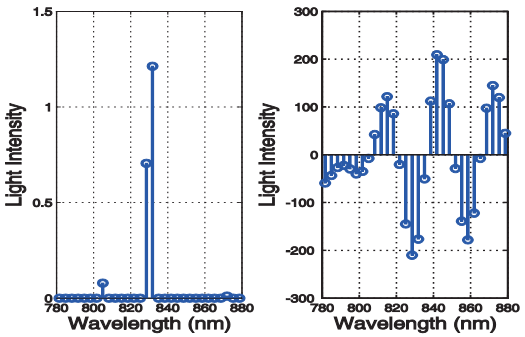

Fig. 1. Estimated signal spectrum in sparse domain (a) Using proposed algorithm (b) Using conventional technique [2].

It is evident from Fig. 1(a) that the dominant spectral components are clearly resolved by the proposed algorithm. However, two additional spectral components appear at 805.02nm and 871.97nm which do not affect the resolvability of the dominant spectral components. Since the two spectral components that are $\Delta\lambda_N$ apart from each other are distinctly resolved with the value of $\mu_N = 1$, the maximum spectral resolution obtained by using $N = 240$ is $\Delta\lambda_{\max} = 3.33\text{nm}$ which is 6 times better than the conventional limit of 20nm assuming $\mu_M = 1$. It is also evident from Fig. 1(b) that the conventional technique provides non-sparse solutions and cannot resolve the two closely spaced spectral components. Based on these results and observations, we conclude that the proposed algorithm outperforms the conventional algorithm in terms of the resolution and our proposed algorithm achieved 6-times improved resolution.

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