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Depth IR spectroscopic data resolution improvement for antibiotics component analysis in critically ill elderly patients

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ABSTRACT

Critically ill patients in intensive care units are vulnerable to the bacterial infections, especially if those patients are elderly. The effective utilization of the appropriate drug can reduce the mortality rates in these patients. Overlap bands often appear in applications of infrared (IR) spectroscopy, for instance in the identification of the unknown material or drugs. This paper considers the problem of noisy and overlapped IR spectroscopic data resolution improvement. A resolution improvement approach with ridgelet transform regularization for IR spectroscopic data and total variation regularization for the apparatus response function. Moreover, the split Bregman method is exploited to solve the resulting minimization problem. It is computationally simple and suitable for implementation on small computers with less memory requirements. Simulation experimental results demonstrates the excellent performance of the proposed approach at noise suppression and spectral detail preserving. The proposed method can remove the random noise and improve the spectroscopic data resolution, thus leading the high-resolution IR spectroscopic data a more efficient tool for component analysis of the unknown antibiotics or drug in critically ill elderly patients.

1. Introduction

Medical studies indicate that the pathological changes in the patients can often influence the body surface temperature. Critically ill patients in intensive care units (ICU) are at high risk of bacterial infections, especially if the patients are elderly. Infrared (IR) spectral analysis appears in various applications such as rapid identification of chemical drugs [1], analytical techniques biomedicine [2,3], and anitbiotics component analysis (ACA) [4,5], etc. Unfortunately, the existence of bands overlap and random Gaussian noise (Fig. 1) in spectroscopic data limits the precision of the feature extraction and spectrum identification [6–8], such as IR spectral feature exaction [9–11], target detection [12–17], and multispectral remote sensing images [18–23]. The experimental apparatus function must be a convolution of many factors, such as slit function, grating response, and circuit response, etc. There are many reasons for the IR spectroscopic noise, mainly including the noise caused by tiny changes of IR light source intensity, the noise caused by stray light, vibration noise caused by external interference, the noise caused by interferometer mirror movement, and circuit noise, etc.

It is critical to reduce the noise in the infrared spectroscopic data and improve its resolution (Fig. 2) before the subsequent spectrum and interpretation processes. It aims to reconstruct a high quality spectrum $\boldsymbol{x}(v)$ from the degraded spectrum $\boldsymbol{u}(v)$ [24–26]. Mathematically, the process of IR spectroscopic data degradation can be generally modeled by

$$\boldsymbol{u}(v) = \boldsymbol{x}(v) \otimes \boldsymbol{h}(v) + \boldsymbol{\eta}(v) \tag{1}$$

where $\otimes$ is convolution product $\boldsymbol{x}(v) \otimes \boldsymbol{h}(v) = \sum_i \boldsymbol{h}_i \boldsymbol{x}(v-i)$, the symbol $\boldsymbol{u}(v)$ denotes the acquired noisy spectroscopic data, matrix $\boldsymbol{H}$ represents the apparatus response function (ARF), $\boldsymbol{h}(v)$ is its vector form. And $\boldsymbol{x}(v)$ denotes the unknown IR spectroscopic data to be estimated; $\boldsymbol{\eta}(v)$ is the additive random noise.

It is well-known that the spectroscopic data reconstruction is a typical ill-posed inverse problem [27,28]. In general, the solution of Eq. (1) is not unique, since small perturbations in the acquired noisy spectroscopic data, due to noise, can cause large variations in the solution. A standard approach for solving an inverse problem is to express

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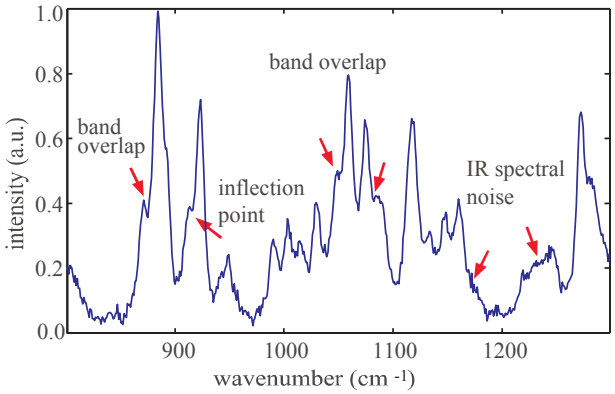

Fig. 1. Infrared spectroscopic data analysis. IR spectroscopic data often suffers from the issues of band overlap and random noise for anitbiotics component analysis.

the desirable solution (*prior* knowledge) as the minimizer of a regularization cost functional. Usually, regularization terms can perfectly model the *prior* knowledge in the following framework,

$$L(\boldsymbol{x}(v), \boldsymbol{h}(v)) = \underset{\boldsymbol{x}(v),\boldsymbol{h}(v)}{\text{Min}} \|\boldsymbol{x}(v) \otimes \boldsymbol{h}(v) - \boldsymbol{u}(v)\|_2^2 + \alpha_1 Reg(\boldsymbol{x}(v)) + \alpha_2 Reg(\boldsymbol{h}(v)) \quad (2)$$

where the first term $\|\boldsymbol{x}(v) \otimes \boldsymbol{h}(v) - \boldsymbol{u}(v)\|_2^2$ is the data fidelity term, which stands for the fidelity between the acquired noisy spectroscopic data and original clean one. In the first term $\|\boldsymbol{x}(v) \otimes \boldsymbol{h}(v) - \boldsymbol{u}(v)\|_2^2$, the subscript 2 and superscript 2 denote the L_2 norm and square operation. Both $Reg(\boldsymbol{x}(v))$ and $Reg(\boldsymbol{h}(v))$ are the regularization terms, denote *a prior* model of the original IR spectroscopic data $\boldsymbol{x}(v)$ and ARF $\boldsymbol{h}(v)$, respectively. The symbols α_1 and α_2 are the regularization parameters, which control the tradeoff between the data fidelity and regularization terms.

Based on Eq. (2), both $Reg(\boldsymbol{x}(v))$ and $Reg(\boldsymbol{h}(v))$ have been specified in different manners, and many IR spectral resolution improvement algorithms have been proposed [29–34]. According to the *priori* knowledge, those methods can be summary as two groups: spatial points-based regularization (SPBR) method and frequency coefficient-based regularization (FCBR) method. For the SPBR methods, the priori knowledge is considered in spatial domain, such as Monte-Carlo approach [35], total variation-based (TV) methods [29,36], and spectral semi-blind deconvolution (SSBD) method [32,37–40]. Liu *et al.* proposed a novelty spectroscopic data resolution enhancement algorithm with the Huber-Markov regularization [41] and achieved impressive results. Then, some other approaches are developed [42], such as maximum entropy deconvolution [28,43], modified minimum entropy deconvolution [25,44], dictionaries learning [26,45,46] and detail-preserving regularization [24,47]. Zhu *et al.* [32] proposed a semi-blind spectral resolution improvement method, in which the ARF is parametrically formulated as a Gaussian shape function. All those methods have achieved the impressive results. In recent years, spectral denoising and reconstruction based on TV regularization [48–51] has been attracting more attention [52–58]. It has been proved that the TV algorithm is a very effective denoising approach, since its effectiveness in preserving spectral features.

For the FCBR methods, the *priori* knowledge is considered in frequency domain. To suppress the staircasing artifacts created by TV-based models, detail-preserving methods such as sparse representations are introduced in spectral reconstruction approaches. A wide variety of transform functions have been proposed, e.g., Fourier [59], wavelet [60], and contourlet [61–63], under the assumption that IR spectroscopic data are usually sparse in an appropriate transform domain. Toth and Mason [64] *et al.* proposed a new low cost, short range, positioning system based on adaptive finite impulse response (FIR) filtering and time domain spectral estimation. For example, Kauppinen *et al.* [65,66] proposed a Fourier self-deconvolution (FSD) algorithm, and proposed a hybrid wavelet-FSD [31] noise reduction approach. In these methods, the assumption is usually made that the ARF is known. In fact, the ARF is difficult to be accurately measured [67]. The apparatus response function is changed as the instrument aging. Especially, it is also affected by the temperature and pressure of experimental environment for anitbiotics component analysis.

Recently, the ridgelet transforms approaches [5] for signal representation can significantly improve signal resolution, since the ridgelet transforms can explicitly exploits the sparse approximations of IR spectroscopic data and can effectively preserves spectral details. Inspired by the consideration, an attempt is made to employ the ridgelet transform regularization to descript the smoothness of IR spectroscopic data. In this article, we develop a new approach for IR spectroscopic data resolution improvement. The approach does not need a known ARF in advance. This approach can effectively make use of the characteristics of ridgelet transforms and produces the desired results. The major novelty of the proposed method is that it can estimate the ARF and latent IR spectroscopic data simultaneously. The main ideas and contributions of the proposed method are summarized as follows:

(1) Ridgelet transforms regularization is studied to handle the IR spectroscopic data resolution improvement issue. The proposed method can effectively remove random spectral noise and preserve structural details via ridgelet regularization.
(2) The split Bregman iteration optimization algorithm is utilized to optimize the proposed IR spectroscopic data resolution improvement model, in which the optimization of the reconstruction model is split into two sub-problems, which can be easy to calculate.

The remainder of this paper is organized as follows. Section 2 formulates the infrared spectroscopic data characteristics and introduces the proposed method. Then the split Bregman method is applied to solve the objective optimization problem in Section 3. In Section 4, the performance of the proposed methods is verified by reconstructing simulated degraded IR spectroscopic data and actual experimental IR spectra. Section 5 draws the final conclusion.

2. Resolution improvement model with discrete ridgelet transform regularization model

2.1. Discrete ridgelet transform regularization

Firstly, the ridgelet transform is employed to analyze the different between the degraded spectroscopic data and high-resolution one. Fig. 3(c) and (d) demonstrate the histogram statistic of the ridgelet coefficients of IR spectroscopic data in Fig. 3(a) and (b). $\boldsymbol{R}$ represents the ridgelet transform using the filters of the ridgelet system. For simplicity, $\boldsymbol{Rx}(v)$ is used to denote the ridgelet coefficient. It finds that the distribution of ridgelet coefficient in Fig. 3(d) is sparser than that in Fig. 3(c). Most coefficients in Fig. 3(d) are close to the value 0. This is because large ridgelet coefficients occur wherever there are singularities such as band shoulder (spectral structure regions, see Fig. 3(d)) and detail information. The ridgelet-based approach essentially keeps large ridgelet coefficients, and thus it preserves spectral structure and detailed information. This motivates us to apply the discrete ridgelet transform regularization to IR spectroscopic data reconstruction. Namely, it can be constructed as

$$Reg(\boldsymbol{x}(v)) = \alpha \|\boldsymbol{Rx}(v)\|_{TV} \quad (3)$$

which penalizes the L_1-norm of the ridgelet transform coefficients of the IR spectroscopic data $\boldsymbol{x}(v)$

A simple schematic diagram for the ridgelet coefficient adjustment is shown in Fig. 3(c)–(d). For the flat region, the low-frequency components should be increased. For the noise region, the mid-frequency components should be decreased. For the shoulder region, the high-