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Deconvolution methods based on convex regularization for spectral resolution enhancement☆

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ABSTRACT

Spectral resolution enhancement is essential for spectral analysis and assignment. In this study, a regularization term in form of a convex function φ_{HS} is included in the spectral deconvolution model to enhance spectral resolution. Based on the regularization term, a non-blind deconvolution (NBD) method is proposed, and to improve feasibility in practice, a semi-blind deconvolution (SBD) method is also presented. Simulation and experimental results demonstrate that both methods enhance spectral resolution effectively. When the blur kernel is known accurately, NBD achieves better performance than SBD. In other cases, the latter achieves better results.

1. Introduction

Generally, the resolution of recorded spectral data is low because measurements with spectrometers often suffer from band overlapping caused by broadening effects of the instrument response function [1,2]. Since low resolution always affects spectral analysis and assignment negatively. Therefore, spectral resolution enhancement technology has attracted more and more attention [3]. Deconvolution, one of the effective methods, has been widely used to solve this problem.

Deconvolution methods are always to be divided into non-blind deconvolution (NBD), blind deconvolution (BD) and semi-blind deconvolution (SBD). NBD methods, e.g., Wiener filtering [4], Fourier deconvolution (FSD) [5], and maximum Burg's entropy deconvolution (MaxEntD) [6], can be widly used and obtain great results when the blur kernel is known accurately. However, the precondition of knowing the blur kernel accurately can not be always satisfied in practical applications. A wrong blur kernel will result in poor deconvolution results. Therefore, the application of NBD methods is restricted. To some degree, the application of BD methods is reasonable because they do not need to know the blur kernel. In [1], a BD method was proposed to estimate the spectrum and blur kernel. In [7], a spectral BD method based on homomorphic filtering was presented. Sarkar et al. introduced a BD method for spectral peak restoration [8]. In [9,10], Yuan et al. proposed a high-order cumulant- and a high-order statistics-based BD method. In [11], Liu et al. presented a BD method based on dictionary learning regularization. These methods can achieved good deconvolution results, but the majority need to estimate the spectrum and the blur kernel simultaneously from the measured data. The unknown blur kernel makes BD a

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complicated and challenging task, and noise complicates it even more. In general, the accurate kernel cannot be known a priori, but the blur kernel shape can be approximately determined. Based on this fact, the SBD method was proposed [12], which assumes that the blur kernel shape is known, but still includes unknown parameters. Further, SBD methods based on different regularization strategies, e.g., φ_{HL} regularization [13], least trimmed squares regularization [14], detail-preserving regularization [15], and others [16,17], were proposed. These methods have achieved good performances regarding spectral resolution enhancement. Compared with BD and NBD, SBD does neither need to estimate the spectrum and blur kernel simultaneously nor does it have need to know the blur kernel accurately. Therefore, SBD is more applicable than NBD and less complex than BD.

The main contributions of this paper are as follows. First, a convex function φ_{HS} is presented, and its advantages as a detail-preserving and noise-suppressing regularization term are explained. Second, based on the φ_{HS} regularization, a spectral NBD model is proposed with the assumption that the blur kernel is known. To make it feasible to resolve spectral data with varying degradation degrees using the spectral deconvolution model, SBD with φ_{HS} regularization is proposed. Herein, the blur kernel is modeled as a parametric form with known shape and unknown parameter. The parameter can be estimated adaptively by using SBD to resolve the degraded spectra. We just need to estimate the spectra and parameters of the blur kernel. The remainder of this paper is organized as follows. Section 2 introduces the basic theory of spectral deconvolution. Section 3 presents the models for enhancing spectral resolution. In Section 4, the performance of the proposed methods is verified by deconvolving simulated degraded spectra and an experimental Raman spectrum. Finally, we draw conclusions in Section 5.

2. Spectral deconvolution model

The measured spectra can be expressed as [13]

$$\mathbf{s} = \mathbf{f} * \mathbf{h} + \mathbf{n} \tag{1}$$

where **s, f** and **n** are vectors representing spectral data of measured spectra, resolved spectra, and noise, respectively, **h** represents the blur kernel vector. In general, presenting only measured spectra **s** to resolve spectra **f** is an ill-posed problem. Therefore, regularized methods are always used to achieve a rather good estimation of **f** [6]. The cost function of spectral deconvolution with the regularization term is given as

$$E(\mathbf{f}) = \frac{1}{2}\|\mathbf{f} * \mathbf{h} - \mathbf{s}\|^2 + \alpha \sum_{i=1}^{N} \varphi(|\mathbf{f}'_i|) \tag{2}$$

where $\sum_{i=1}^{N} \varphi(\left|\mathbf{f}'_i\right|)$ represents the regularization term, $|\mathbf{f}'|$ is the absolute value of the first derivative of **f**, N is the number of data points of the test spectrum, and α is a regularization parameter. The minima of Eq. (2) can be obtained based on the Euler-Lagrange equation using Neumann boundary condition.

3. Proposed models

3.1. φ_{HS} regularization

In [18–20], the convex function named φ_{HS} is mentioned and used in image processing for edge preservation. In this paper, we define a convex function

$$\varphi_{HS}(\left|\mathbf{f}'\right|) = \sqrt{1 + |\mathbf{f}'|^2} - 1 \tag{3}$$

Since it has the same form as the φ_{HS} function mentioned in refs. [18–20], we also called it the φ_{HS} function.

Since spectral details such as steep regions are smoothed during the deconvolution, it is necessary to introduce a regularization term for detail preservation and noise suppression. Therefore, the φ_{HS} function is included in the spectral deconvolution model.

The advantages of using the φ_{HS} as regularization term are given as follows:

Firstly, the weighting function [13] corresponding to φ_{HS} is given as

$$\frac{\varphi'_{HS}(|\mathbf{f}'|)}{|\mathbf{f}'|} = \frac{1}{\sqrt{1 + |\mathbf{f}'|^2}} \tag{4}$$

It is obviously that the weighting function $\frac{\varphi'_{HS}(|\mathbf{f}'|)}{|\mathbf{f}'|}$ smooths noise while preserving details, as given in Ref. [13].

Secondly, φ_{HS} has been successfully used in image processing for edge preservation [20], and there exist similarities between the image gradient and the spectrum derivative. For instance, image gradients are small in homogeneous areas while they are large near the edges. Spectrum derivatives are also small in flat spectral regions while they are large in steep regions.

Lastly, φ_{HS} is a convex function that can ensure the existence and uniqueness of a solution for the minimization problem [20].