Adaptive Regularization Deconvolution Extraction Algorithm for Spectral Signal Processing

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Abstract—Deconvolution is known as an ill-posed problem. In order to solve such a problem, a regularization method is needed to constrain the solution space and find a plausible and stable solution. In practice, it is very computation intensive when using cross-validation method to select the regularization parameter. In this paper, we present an adaptive regularization method to find the optimal regularization parameter value and represent the trade-off between model fitness of the data and the smoothness of the extracted signal. Spectral signal extraction experimental results demonstrate that the time complexity the proposed method is much lower than that of current deconvolution extraction method and other extraction method used in the Large Area Multi-Objects Fiber Spectroscopy Telescope spectral signal processing pipeline.

I. INTRODUCTION

In the field of digital image processing, image restoration problem represents one of the primary research focuses. Degradation is hard to avoid in any image acquisition systems, such as astronomical telescope, remote sensing and medical imaging which is caused not just by only one source but by many, such as atmospheric turbulence, an out-of-focus optical system and aberrations in the imaging system, and so on. The degradation can be described as a convolution of the original image with a point spread function (PSF)\cite{1} and some noise. While to recover the original image is an inverse problem in mathematics, deconvolution is a crucial method for the inverse problem \cite{2}\cite{3}, which aims to recover an estimate of the original image from the degraded observations.

Deconvolution is known as an ill-posed problem, this means that there is no unique and stable solution. And we need to introduce regularization to constrain the solution space and find a plausible and stable solution. Some techniques such as cross-validation (CV) \cite{4}\cite{5} are utilized to find the optimal regularization parameter value. The CV method works well, but it is computational intensive in practice.

In this work, an adaptive regularization method is presented to find the optimal regularization parameter value adaptively and represents the trade-off between model fitness of the data and the smoothness of the extracted signals. For validating the proposed method, spectral signal extraction experiments for multi-objects fiber spectroscopy charge-coupled device (CCD) images are used.

The article is organized as follows. The proposed method is described in Section 2. In Section 3, experiments and results discussion are given. A conclusion is presented in the last section of this paper.

II. METHOD

A. Mathematical Formulation

Mathematical expression for image restoration can be described as follows.

Let $x(i,j)$ be the true two dimensional intensity distribution which is referred as the true image, where $i,j$ are orthogonal coordinates in the image. The standard integration model for the description of the degraded image is as follows:

$$b(i,j) = \int \int h(i-k,j-l)x(k,l)dldj + \varepsilon(i,j).$$

(1)

Where $b$ is the observed (or degraded) image, $h$ is the spatially invariant point spread function (PSF), and $\varepsilon$ represents the additive noise in the data.

A discrete model of Equation (1) is usually formulated by a large-scale linear system:

$$b(i,j) = \sum \sum h(i-k,j-l)x(k,l) + \varepsilon(i,j).$$

(2)

Equation (2) can be expressed as the following matrix form:

$$b = Ax + \varepsilon.$$  

(3)

Where $A$ is a convolution matrix defined by the PSF.

Let the size of PSF be $(2 \times m + 1)$ where $m$ is a positive integer and the form of PSF can be depicted as follows:

$$H = \begin{pmatrix}
    h(-m,-m) & \cdots & h(-m,0) & \cdots & h(-m,-m) \\
    \vdots & \ddots & \vdots & \ddots & \vdots \\
    h(0,m) & \cdots & h(0,0) & \cdots & h(0,-m) \\
    \vdots & \ddots & \vdots & \ddots & \vdots \\
    h(m,m) & \cdots & h(m,0) & \cdots & h(m,-m)
\end{pmatrix}.$$
Where \( h_{(0,0)} \) is the center of the PSF array. Convolution matrix \( A \) can be obtained by expanding \( H \). In this paper, the boundary conditions are supposed to be zero boundary conditions[6]. In this case, the form of \( A \) is shown as follows:

\[
A = \begin{pmatrix}
    T(0) & \cdots & T(-m) & 0 \\
    \vdots & & \vdots & \vdots \\
    T(m) & \cdots & T(-m) & 0 \\
    0 & T(m) & \cdots & T(0)
\end{pmatrix}
\]

Where \( A \) is a block-Toeplitz matrix[6] and \( T \) is a Toeplitz matrix [1].

Taking \( T(0) \) as an example, and omit same subscript 0 in \( h_{(0,m)} \), the form of \( T(0) \) is shown as follows:

\[
T(0) = \begin{pmatrix}
    h(0) & \cdots & h(-m) & 0 \\
    \vdots & & \vdots & \vdots \\
    h(m) & \cdots & h(-m) & 0 \\
    0 & h(m) & \cdots & h(0)
\end{pmatrix}
\]

Usually matrix \( A \) is not a square matrix and severely ill-conditioned. To obtain \( x \) by deconvolution algorithm is a typically ill-posed problem. Therefore, we have to obtain the solutions with the use of the least squares method to minimize \( \|b - Ax\|_2 \). While the additive noise \( \varepsilon \) in the image may give rise to significant errors in the above computation, a regularization technique is needed to obtain the stable solutions.

The least square solution of \( x \) with regularization method can be expressed as minimizing following equation:

\[
\|Ax - b\|_2 + \eta \|x\|_2, \tag{4}
\]

where \( \eta \) is the regularization parameter and greater than or equal to zero and less than 1.

Iterative methods such as conjugate gradient type approaches can be applied for solving this deconvolution problem. On considering the characteristics of the convolution matrix \( A \), sparse, large-scale and ill-posed, here we can utilize the LSQR algorithm to solve this least square problem of the equation (4).

**B. LSQR Algorithm**

For this kind problem, some algorithms such as Cholesky decomposition, LU decomposition and QR decomposition cannot be applied to solve this sparse linear equations. Singular value decomposition (SVD) requires more memory usage. Least squares conjugate-gradient (LSCG) algorithm does not perform well when the convolution matrix \( A \) is large-scale and ill-conditioned.

Therefore, we adopt regularized (or damped) LSQR [7][8] [9] which introduces a regularization parameter \( \eta \). Then our aim is to solve the damped least squares, namely, minimize equation (4) to find least square solution.

In order to illustrate our adaptive regularization technique conveniently, the pseudo code for the solution of \( x \) using regularized LSQR are described as follows:

1) Initialize.
   \[
x(0) = 0, \quad u_0 = b, \quad \beta_0 = \|u_0\|_2, \quad \varphi_0 = \eta_0, \quad v_0 = A^T u_0, \quad \alpha_0 = \|v_0\|_2, \quad p_0 = \alpha_0.
\]

2) For \( i = 1, 2, 3, \ldots \), repeat steps 3-6.

3) Continue the bi-diagonalization.
   \[
u_{i+1} = A v_i - \beta_i u_i, \quad \alpha_{i+1} = \|v_{i+1}\|_2, \quad v_{i+1} = A^T u_{i+1} - \beta_{i+1} v_i, \quad \beta_{i+1} = \|v_{i+1}\|_2.
\]

4) Construct and apply next orthogonal transformation (QR-factorization).
   \[
   p_{i+1} = \|v_{i+1}\|_2, \quad \varphi_i = \frac{\|v_{i+1}\|_2}{\|v_i\|_2}, \quad \rho_i = \|p_{i+1}\|_2, \quad \varphi_i = \frac{\|v_{i+1}\|_2}{\|v_i\|_2}, \quad \alpha_{i+1} = \|v_{i+1}\|_2.
\]

5) Update \( x, w \).
   \[
x_{i+1} = x_i + w_i \frac{\|v_{i+1}\|_2}{\alpha_i}, \quad w_{i+1} = v_{i+1} - w_i \frac{\|v_{i+1}\|_2}{\alpha_i}.
\]

6) Test for convergence, exit if some stopping criteria have been met, otherwise goto step (3).

In this work, the stopping criteria for the algorithm is that the algorithm running reach the maximum iteration or the residual \( r \) changes less than \( 10^{-22} \) for successive 3 iterations. In above iterative steps, \( x(0) \)’s initial value is zeros. And \( u_0 \)'s initial value is derived from vector \( s \). The other variables including \( \alpha_i, \beta_i, \varphi_i, \rho_i, \varphi_i, \rho_i \) are intermediate variables during the processing of algorithm.

\( x(i) \) is the solution at \( i \)-th iteration during the processing of LSQR. Let \( n \) be the number of convergence iteration, \( x(n) \) is the final solution. The reasons for fast computation of least squares solution are that LSQR algorithm only involves multiplication of matrix and vector, and nonzero value’s calculation. That can save memory usage and speed up calculation greatly. Therefore, LSQR algorithm is especially suitable for the solution of large-scale sparse linear equations.
Furthermore, the PSF we adopted has a symmetry and convolution matrix $A$ expanded by this PSF has Toeplitz symmetry too. In fact, LSQR algorithm can solve the least squares problem accurately and efficiently because it only requires convolution matrix being sparse but not requiring Toeplitz symmetry property. In other words, there is no influence for the solution to the problem with LSQR algorithm even Toeplitz symmetry was broken.

C. Adaptive Regularization Technique

Generally, the choice of an appropriate regularization parameter $\eta$ can be evaluated empirically, or cross-validation algorithm be used. However, in practice it is very difficult to select a proper regularization parameter with empirical method. Also, if using the CV method, it is computation intensive for this large-scale problem. In our previous research work, we have done a theoretical analysis for selecting the regularization parameters [10][11][12]. These theoretical research results show that the regularization parameter has some kind relationship with the objective function. In our study, $\overline{\varphi}$, this scalar which is derived from $\overline{\varphi}$ is utilized as the objective function, where $\overline{\varphi}$ represents the diagonal of the lower-bidiagonal matrix. Hence the regularization parameter would be expected to be related to $\overline{\varphi}$. Furthermore, the value of regularization parameter is required to vary with $\overline{\varphi}$. That is to say, a greater regularization parameter value is needed for a larger error during iterations. If the $\overline{\varphi}$ is very low, only a small regularization parameter value is needed to regularize the ill-posed process.

Based on these considerations, we propose that the regularization parameter $\eta$ is estimated adaptively as follows:

$$\eta = \frac{1}{1 + e^{-\overline{\varphi}}}.$$ (5)

In equation (5), the regularization parameter $\eta$ varies in the range from 1/2 to 1. It includes three primary considerations:

1) Due to the ill-posed characteristic of the inverse problem, the regularization should not be reduced with iterations to too small of a value.
2) The regularization value should be quantitatively similar to the diagonal of the matrix $(A^T A)^{-1}$.
3) Equation (5) for the regularization parameter $\eta$ does not includes any empirical coefficients, so equation (5) is convenient for users.

III. Experiments & Discussions

Deconvolution method has been proven to be effective for extracting scientific content [13], which can be applied to extract spectral signal in CCD images [14]. In this part, we use our proposed deconvolution method with adaptive regularization (D-AR) method to extract spectral lines from a raw 2D arc-lamp CCD image and a raw 2D flat-field CCD image, these images are obtained in Large Area Multi-Objects Fiber Spectroscopy Telescope (LAMOST). A section (301×30 pixels in size) of a raw 2D arc-lamp CCD image is shown in Figure (1) and a section (301×30 pixels in size) of a raw 2D flat-field CCD image is shown in Figure (2). We also compared the D-AR algorithm with other deconvolution methods when applied to spectral signal processing.

$$h(i,j) = \frac{\alpha}{\sqrt{2\pi|\Sigma|}} \exp \left[ -\frac{1}{2} (i,j) \Sigma^{-1} \left( \begin{array}{c} i \\ j \end{array} \right) \right],$$ (6)

where

$$\Sigma = \begin{pmatrix} \sigma_i^2 & \sigma_{ij} \\ \sigma_{ji} & \sigma_j^2 \end{pmatrix}.$$
For computing simplicity consideration, in this paper we only consider the case \( \sigma^2_{ij} = 0 \), will adopt the following modified Gaussian PSF experientially:

\[
\mathbf{h}(i, j) = \frac{\alpha}{\sqrt{2\pi} \sigma_i \sigma_j} \exp \left[ -\frac{1}{2} \left( \frac{i^2}{\sigma_i^2} + \frac{j^2}{\sigma_j^2} \right) \right].
\] (7)

Where \( i \) and \( j \) are the offsets in pixels on the CCD image from the center of the PSF spot in the wavelength and space direction, respectively. Here, \( \sigma_i \) and \( \sigma_j \) controls the size of the Gaussian kernel from wavelength direction and space direction, respectively. That is to say, these two parameters determine the ellipticity of the shape of Gaussian PSF.

For the purpose of illustrating the accuracy of deconvolution extraction spectrum line method, hence, we compare our proposed method with the boxcar (aperture) method [15][16] which is utilized in LAMOST spectrum processing pipeline. The boxcar method makes a box (aperture) which is bounded by midpoints between the two adjacent fiber profile around each fiber, and gains the flux value of a fiber in this row by simple summing the pixels enclosed by the box. boxcar method is very easy to use, but it has two limitations, fiber-to-fiber crosstalk and damage of the noise pixels, to restrict extraction spectrum accuracy. While deconvolution method can deal with the fiber-to-fiber cross talk problem well [13].

We take the advantage of our research results and convert spectrum extraction into the image restoration problem. Following experimental results show that the proposed deconvolution method with adaptive regularization (D-AR) method has better performance than that either boxcar method or deconvolution method without regularization.

Parts of a 2D arc-lamp CCD image extraction results are shown in Figure (3) – (6), while parts of a 2D flat-field CCD image extraction results are shown in Figure (7) – (10).

To further comparing our proposed D-AR method with the boxcar extraction method when applied to 2D raw arc-lamp CCD images and 2D raw flat-field CCD images, we give out the quantitative performance analysis with the root mean square error (RMSE) for the extraction spectrum comparing with theoretical model spectrum.

The RMSE of the spectrum extraction methods can be expressed as follows:

\[
\text{RMSE} = \frac{\| \mathbf{f}_{\text{origin}} - \mathbf{f}_{\text{extracted}} \|_2}{\sqrt{n}},
\] (8)

where \( \mathbf{f}_{\text{extracted}} \) is the flux extracted by the spectrum extraction method, \( \mathbf{f}_{\text{origin}} \) is flux of the original spectrum, and \( n \) is the length of \( \mathbf{f} \).

The RMSE of arc-lamp spectrum extraction results is shown as Table (I), and the RMSE of flat-field spectrum extraction results is shown as Table (II).
In deconvolution method, usually the exhaustion search algorithm is used to search a proper regularization parameter \( \eta \), its time complexity is \( O(n^3) \). While using our proposed adaptive regularization method in deconvolution, the regularization parameter \( \eta \) adaptively estimated with \( \varphi \) at each iteration. Consequently, the time complexity of D-AR method is \( O(n^2) \).

Same as problem encountered in image restoration, when using deconvolution method to extract 1D spectra will encounter the ringing effects also. The ringing effects generated by deconvolution at least include the following two cases: (1) Caused by inaccurate PSF, especially the size of PSF extraction with adaptive regularization method. We consistently observed our proposed D-AR method to perform better than boxcar and deconvolution extraction method. And the D-AR method can reach the minimum error. It also illustrates that the proposed method has the best spectrum extraction accuracy.

### Table I. RMSE of Arc-Lamp Spectrum Extraction

<table>
<thead>
<tr>
<th>Fiber</th>
<th>Boxcar</th>
<th>Deconvolution</th>
<th>D-AR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>367.59</td>
<td>219.56</td>
<td>166.92</td>
</tr>
<tr>
<td>3</td>
<td>497.48</td>
<td>162.69</td>
<td>139.57</td>
</tr>
<tr>
<td>10</td>
<td>658.95</td>
<td>148.22</td>
<td>142.21</td>
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<td>657.62</td>
<td>186.13</td>
<td>140.13</td>
</tr>
<tr>
<td>25</td>
<td>675.03</td>
<td>225.57</td>
<td>171.48</td>
</tr>
</tbody>
</table>

### Table II. RMSE of Flat-Field Spectrum Extraction

<table>
<thead>
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<th>Boxcar</th>
<th>Deconvolution</th>
<th>D-AR</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1537.40</td>
<td>173.23</td>
<td>108.32</td>
</tr>
<tr>
<td>12</td>
<td>1664.15</td>
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</tr>
<tr>
<td>20</td>
<td>1764.87</td>
<td>271.77</td>
<td>95.70</td>
</tr>
<tr>
<td>24</td>
<td>675.03</td>
<td>308.34</td>
<td>159.97</td>
</tr>
</tbody>
</table>
selected is larger than the size of actual one, in this case the ringing effects is more significant. (2) Caused by the border discontinuity of gray level data altering at the edge of image. In this work, we adopted zero boundary conditions to reduce ringing effects. That proves to be effective through experiments. In addition, the essence of LSQR method is the iterative regularization, which is suitable for ill-posed problem and can reduce ringing effects if a proper regularization parameter is selected. In principle, parameter $\sigma$ in PSF can be regarded as a smooth parameter, which has been proved that is equivalent to the regularization parameter in our previous work[10][11]. In this work, we developed an adaptive regularization method to extract spectrum lines, which can reduce the ringing effects also.

IV. CONCLUSION

In this paper, an adaptive regularization algorithm for enhancing the resolution of the deconvolution-based problem is proposed. The proposed method can estimate the regularization parameter adaptively for the solution at each iteration, which is convenient for users and its time complexity is much lower than that the one without adaptive regularization. Quantitative performance analysis of precision with RMSE shows that the proposed intelligent approach performs better than that of current deconvolution extraction method and the extraction method used in the LAMOST spectral signal processing pipeline in real world problem applications.

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