PARAMETER ESTIMATION FOR INSTANTANEOUS SPECTRAL IMAGING

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ABSTRACT

Spectral imaging is a fundamental diagnostic technique in physical sciences with widespread application. Conventionally, spectral imaging techniques rely on a scanning process, which renders them unsuitable for dynamic scenes. Here we study the problem of estimating the physical parameters of interest from the measurements of a non-scanning spectral imager based on a parametric model. This inverse problem, which can be viewed as a multi-frame deblurring problem, is formulated as a maximum a posteriori (MAP) estimation problem. The global optimum of the nonlinear MAP problem is found using an efficient dynamic programming algorithm. Lastly, the method is illustrated for an application in solar spectral imaging. Numerical results suggest that estimation accuracy is comparable to the conventional slit spectroscopy, but with the added benefit of a two-dimensional field-of-view.

1. INTRODUCTION

Observing the spectrum of a radiating scene, known as spectral imaging, is a fundamental diagnostic technique in physical sciences with application in diverse fields such as physics, chemistry, biology, medicine, astronomy, and remote sensing. The measured spectrum is the main source of information about the chemical composition and physical properties of targeted objects. For example, in astrophysical imaging of space plasmas, estimates of the plasma parameters (such as density, temperature, and flow speed of the ions) are inferred from spectral emission line measurements, hence enabling the investigation of the complex plasma behavior [1].

Spectral imaging of a two-dimensional scene requires simultaneously capturing a three-dimensional data (2-D spatial and 1-D spectral) on an inherently 2-D detector. Conventional techniques rely on a scanning process to build up this three-dimensional data from a series of two-dimensional measurements that are acquired sequentially. Spectrometers with long slits, imagers with multiple spectral filters, Fourier and Hadamard transform based spectrometers all work with this principle [2]. As a result, these conventional methods are not suitable for dynamic scenes which evolve on time scales faster than the scanning process involved.

More recently, methods that build up the three-dimensional data cube from a single-shot measurement have been proposed by using coded apertures [3, 4] and tomographic approaches [5–9]. In this work, we consider a different instantaneous (non-scanning) spectral imaging technique with a parametric approach [11, 12], which is specifically aimed for dynamic scenes encountered in space remote sensing. Figure 1 shows the schematic depiction of the system involved. In contrast to a slit spectrometer, the input to this system is a two-dimensional image of the scene (from a telescope), and the output is multiple spectrally dispersed images of the scene in different diffraction orders.

Fig. 1: Schematic view of the instantaneous spectral imager with three diffraction orders 0, +1, and -1 (i.e. three detectors)

In this paper, we study the problem of estimating the physical parameters of interest from the measurements of this snapshot spectral imager by using a parametric model for the measurements. We formulate this inverse problem as a maximum a posteriori (MAP) estimation problem by incorporating the prior knowledge of the physical parameters of interest. The global optimum of the nonlinear MAP problem is found using an efficient dynamic programming algorithm, which is an extension of a previously proposed algorithm for maximum likelihood parameter estimation of superimposed signals [13, 14]. Lastly, we illustrate the performance of the algorithm for an application in solar spectral imaging.

Our previous work had focused on performing a Cramer-Rao bound analysis [11, 12] demonstrating that the estimation accuracy can be comparable to the conventional slit spectroscopy, while enabling a two-dimensional FOV at the same time. The inversion results of this paper validate this finding.

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2. FORWARD PROBLEM

Dispersed images can be modeled parametrically in astrophysical imaging of space plasmas [10–12]. In this parametric model, each spatial pixel \( m \) in the scene produce a dispersed spectral line that has a Gaussian shape, and is characterized by three parameters of interest: integrated line intensity \( f_m \), line width \( \Delta_m \), and line center shift (Doppler shift) \( \epsilon_m \). In the dispersed image, the spectral lines from all pixels are superimposed. Considering a row of pixels of length \( M \), this superposition can be mathematically expressed as

\[
y_a^m = \sum_{m' = 1}^{M} f_{m'} \phi^a(m - m'; \Theta_{m'}),
\]

where \( y_a^m \) is the intensity of the \( a \)-th order dispersed image at pixel \( m \), superimposed signal \( \phi^a(m - m'; \Theta_{m'}) \) with \( a \neq 0 \) is a unit Gaussian line profile arising from pixel \( m' \), and \( \Theta_{m'} = [\epsilon_{m'}, \Delta_{m'}]^T \). Line widths \( \Delta_{m'} \) and center shifts \( \epsilon_{m'} \) are measured in pixel units, and in the first diffraction order \( (a = +1) \). For higher orders, these are scaled by the spectral order \( a \).

Let us define the vectors \( y_a = [y_1^a \ldots y_M^a]^T \), \( f = [f_1 \ldots f_M]^T \), \( \epsilon = [\epsilon_1 \ldots \epsilon_M]^T \), and \( \Delta = [\Delta_1 \ldots \Delta_M]^T \). Based on this model, each dispersed image \( y_a \) can be viewed as a blurred version of the same object \( f \) with a different spatially-varying (Gaussian) filter of some unknown parameters \( \epsilon \) and \( \Delta \) [11, 12]. Also when the order is zero, there is no dispersion and hence no blur on the image, i.e., \( y_0 = f \).

For any order \( a \), the complete observation model with noise is given in vector-matrix form, by

\[
\tilde{y}^a = H^a(\Theta) f + n^a,
\]

where \( H^a(\Theta) = [h^a(1; \Theta_1) \ldots h^a(M; \Theta_M)] \) with \( \Theta = [\Theta_1 \ldots \Theta_M] \) and \( h^a(m'; \Theta_{m'}) = \phi^a(1-m'; \Theta_{m'}) \ldots \phi^a(M - m'; \Theta_{m'}) \), and \( n^a = [n_1^a \ldots n_M^a]^T \) is the noise vector with each \( n_{m}^a \sim N(0, \sigma^2) \) and uncorrelated across both \( m \) and \( a \).

Let \( A = \{a_1, a_2, \ldots, a_N \} \) be the set of all diffraction orders that are measured. Then by stacking all measured dispersed images into a single vector, \( \tilde{y} \), the model becomes

\[
\tilde{y} = H(\Theta)f + n,
\]

3. INVERSE PROBLEM

In the inverse problem, the goal is to estimate the unknown spectral line parameters \( f \) and \( \Theta \) from the measurements \( \tilde{y} \). We formulate this inverse problem as a MAP estimation problem that incorporates prior knowledge of the statistics of the spectral line parameters. (Such statistics can be obtained from the measurements of existing slit spectrometers.) Treating \( f, \Delta, \) and \( \epsilon \) as independent random vectors, the MAP estimates of \( f, \Delta, \) and \( \epsilon \) from the measurements \( \tilde{y} \) are given by

\[
\arg\max_{f,\Delta,\epsilon} p(\tilde{y} | f, \Delta, \epsilon) \ p(f)p(\Delta)p(\epsilon) \quad (4)
\]

where \( p(\tilde{y} | f, \Delta, \epsilon) \) represents the conditional probability density function (pdf) of \( \tilde{y} \) given \( f, \Delta, \) and \( \epsilon \), and \( p(f), p(\Delta), \) and \( p(\epsilon) \) denote the prior distributions.

Note that the zeroth order image, \( \tilde{y}^0 \), is a noisy observation of \( f \), and hence if it is observed at a sufficiently high SNR, then the effect of a broader prior of \( f \) will be almost negligible. For this reason, we remove \( p(f) \) from the above MAP formulation, which yields to a simpler form of a separable nonlinear least squares problem [15]. For the priors \( p(\Delta) \) and \( p(\epsilon) \), we assume that parameters at different pixels are independently distributed. Lastly, the conditional pdf \( p(\tilde{y} | f, \Delta, \epsilon) \) comes from the noisy observation model in (3). After combining all of these together, and taking the logarithm of (4), the MAP estimation problem becomes

\[
\min_{f,\Delta,\epsilon} \frac{1}{2\sigma^2} ||\tilde{y} - H(\Theta)f||_2^2 + \sum_{m=1}^{M} r(\Theta_m), \quad (5)
\]

where \( r(\Theta_m) = -\log p(\Delta_m) - \log p(\epsilon_m) \) is the regularization functional arising from priors.

4. DYNAMIC PROGRAMMING ALGORITHM

We use an efficient dynamic programming algorithm to find the global optimum of the nonconvex MAP problem. This algorithm is an extension of a robust dynamic programming algorithm that was previously proposed for maximum likelihood parameter estimation of superimposed signals [13, 14].

This algorithm performs an efficient search (equivalent to exhaustive search) by exploiting the special structure of the problem, which is the interaction of superimposed signals (i.e., Gaussian line profiles) with only few of their closest neighbors. Let \( r \geq 1 \) be the number of closest neighbors that each superimposed signal interacts on both sides. Then mathematically, this local interaction model [13] is expressed as

\[
h_i(\Theta_i)^*h_j(\Theta_j) \approx 0 \quad \text{for} \quad |i - j| > r, \quad (6)
\]

implying that the \( i \)th and \( j \)th columns of \( H(\Theta) \), related to \( i \)th and \( j \)th superimposed signals, are approximately orthogonal if they are separated by more than \( r \) columns.

Here we revisit the algorithm [13] and its derivation for a more general setting that involves priors and superimposed signals with interaction \( r > 1 \). When the model in (6) holds, the least squares term in the MAP functional can be approximated as
\[ \| \hat{y} - H(\Theta)f \|^2 \] (7)
\[ \approx \| \hat{y} - H(\Theta_{[k+1:k+r]}f_{[k+1:k+r]} - H(\Theta_{[1:k]}f_{[1:k]}) \|^2 + \| \hat{y} - H(\Theta_{[k+r+1:M]}f_{[k+r+1:M]} - H(\Theta_{[k+r+1:M]}f_{[k+r+1:M]})) \|^2 - \| \hat{y} - H(\Theta_{[k+1:k+r]}f_{[k+1:k+r]} - H(\Theta_{[1:k]}f_{[1:k]})\|^2 \]

where \( \Theta_{[1:2]} \) denotes \( [\Theta, \Theta_{[2]}] \) and likewise \( f_{[1:2]} \).

Then the MAP functional has the generic functional form of
\[ g(x_{[1:M]}) = g_1(x_{[1:M]}, x_{[k+1:k+r]}) + g_2(x_{[k+1:k+r]}, x_{[k+r+1:M]}) \] (8)

with \( x_k = (\Theta, f) \), where the function \( g_1(\cdot) \) contains the first term of (7), and \( g_2(\cdot) \) contains the last two terms of (7), in addition to the prior terms.

This form enables to efficiently find the global minimum of (7) via dynamic programming [16–18]. This is because given \( x_{[k+1:M]} \), the optimal values of \( x_1, \ldots, x_k \) are a function of only \( x_{[k+1:k+r]} \), hence can be denoted as \( x_{[1:k]}(x_{[k+1:k+r]}) \). Then the principle of conditional optimization [18] allows to efficiently solve the high-dimensional problem by solving smaller subproblems that are related to each other recursively. More specifically, if we define the \( k \)th subproblem as finding \( x_{[1:k]}(x_{[k+1:k+r]}), \) then it can be solved by using the solution of the \( (k-1) \)th subproblem:

\[ x_{[1:k]}(x_{[k+1:k+r]}) = \arg \min_{x_{[1:k-1]}} g_1(x_{[1:k]}, x_{[k+1:k+r]}) \] (9)

which performs a search in a reduced set.

Each subproblem can also be simplified. Minimization over \( \Theta_{[1:k]} \) can be solved separately by eliminating \( f_{[1:k]} \) from (9) based on the variable projection technique [15]. Then the \( k \)th subproblem becomes

\[ \min_{\Theta_{[1:k]}} \| P_A^{+}H(\Theta_{[1:k]})[\hat{y} - H(\Theta_{[k+1:k+r]}f_{[k+1:k+r]} - H(\Theta_{[1:k]}f_{[1:k]}))] \|^2 + \sum_{m=1}^{k} r(\Theta_m) \] (10)

where \( P_A^{+} = I - A(A^*A)^{-1}A^* \) is the projection matrix onto the orthogonal complement of the column space of \( A \).

2. Updating \( (k = 2, \ldots, M - r) \):
(a) For each \( (\Theta_{[k+1:k+r]}, f_{[k+1:k+r]}) \in \Omega^r \), solve
\[ \hat{\Theta}_{[k+1:k]}(\Theta_{[k+1:k+r]}, f_{[k+1:k+r]}) = \arg \min_{\Theta_{[1:k]}} \| P_A^{+}H(\Theta_{[1:k]})[\hat{y} - H(\Theta_{[k+1:k+r]}f_{[k+1:k+r]} - H(\Theta_{[1:k]}f_{[1:k]}))] \|^2 + r(\Theta_1) \]
(b) Record the optimal values as a function of \( \Theta_{[2:k]} \):
\[ \Theta^*_{[1:k]}(\Theta_{[2:k]}, f_{[2:k]}) = \{ \Theta_{[1]} \in \Lambda : \Theta_{[1:k]} = \hat{\Theta}_{[1:k]}(\Theta_{[2:k]}, f_{[2:k]}) \text{ for some } f_{[2:k]} \in \Pi' \} \]

3. Final step:
(a) Estimates of \( \Theta \) and \( f \) are given by
\[ \hat{\Theta} = \arg \min_{\Theta_{[M-r+1:M]}} \min_{\Theta_{[1:M-r]} \in \Theta^*_{[1:M-r]}} \| P_A^{+}H(\Theta_{[1:M]})[\hat{y}] - H(\Theta_{[k+1:k+r]}f_{[k+1:k+r]} - H(\Theta_{[1:k]}f_{[1:k]})) \|^2 + \sum_{m=1}^{M} r(\Theta_m) \]
\[ \hat{f} = [H^*(\hat{\Theta})H(\hat{\Theta})]^{-1}H^*(\hat{\Theta})\hat{y} \]

We now revisit the computational requirements of the extended algorithm. Let \( q \) be the number of quantization levels used in exhaustive search for each scalar parameter, and \( n \) and \( p \) be the number of scalar parameters in each \( \Theta_m \) and \( f_m \), respectively. (In our problem, \( p = 1 \) and \( n = 2 \).) Then it can be easily found that the total number of objective function evaluations is of \( O(q^r(2p+n)+n) \). Hence the computational cost is exponential only in the number of interacting signals, \( r \), as opposed to the exponential cost in \( M \) in exhaustive search.

5. Sample Application
We now illustrate the effectiveness of the spectral imaging technique and MAP estimation algorithm for an application in solar spectral imaging [1]. For this, we consider a strong extreme ultraviolet (EUV) solar emission line, with a central wavelength of \( \lambda_0 = 195.12 \) Å.

5.1. Implementation choices for the algorithm
To implement the dynamic programming algorithm, we need to specify the prior distributions, the number of interacting signals, \( r \), the constraint sets for the parameters \( \Theta \) and \( f \), and how to quantize these constraint sets for the numerical search.

We model the line widths and Doppler shifts as independent and identically distributed random variables over pixels. Their prior distributions are estimated from observations
of Hinode satellite’s EUV imaging spectrometer (EIS) [19], which is a slit spectrometer. Figure 2 shows the obtained histograms and fitted Gaussian distributions (shown in red). The fitted distributions are also scaled to convert the parameters in physical units to pixel units [12] by scaling them with the operating dispersion scale (the wavelength range covered by a single pixel).

Noting that the prior distributions of line widths and Doppler shifts are Gaussian, we constrain each parameter to within three standard deviations (std) from its mean. Similarly, noting that \( \tilde{y}_m^0 \) is a noisy observation of \( f_m \) and has Gaussian distribution, we define bounds for \( f_m \) as three noise std from \( \tilde{y}_m^0 \). To quantize this constrained parameter space for exhaustive search, one option is uniform quantization [13] where the number of quantization levels chosen based on the Cramer-Rao error bounds of the parameters [12]. Instead, we choose a nonuniform quantization grid that takes into account the Gaussian distribution of the parameters. A grid is assigned to each region of equal probability, yielding to a denser grid around the mean.

Lastly for the choice of \( r \), we require that

\[
\frac{\| h_i(\Theta_j) \|^2}{\| h_i(\Theta_j) \|^2_{2}} < 10^{-3} \text{ for } |i - j| > r. \tag{11}
\]

We choose the smallest integer value of \( r \) that makes this argument true for all possible \( \Delta_i, \epsilon_i, \Delta_j, \text{ and } \epsilon_j \).

5.2. Numerical results

Measurements of the instantaneous spectral imager are simulated based on the parametric model in (2). For this, spectral line parameters are randomly generated according to their modeled prior distributions. The dynamic programming algorithm is used to estimate the spectral line parameters from the simulated measurements. A gradient-based interior-point algorithm (a local optimization method) is used afterwards in order to refine the resulting estimates (limited by the finite grid size).

Fig. 3 shows a typical result with \( \{0, +1, -1\} \) orders, and at a dispersion scale, \( D \), of 50 mÅ/pixel. The estimated parameters yield estimated observations that are almost same as the given observations. With only three orders, root-mean-square (rms) errors are typically less than 2 for intensities, 1 mÅ for line widths, and 1.5 km/s for Doppler shifts. This estimation accuracy is similar to the accuracy of the state-of-the-art slit spectroscopy used for this application [19], which only have a 1D FOV. Measuring more than three orders helps further to reduce these errors.

Fig. 4 shows the results of 50 Monte Carlo runs at various noise levels, with \( D = 50 \) mÅ/pixel and \( M = 10 \). When the noise std is smaller than 4 (corresponding to an SNR of \( \sim 50 \)), the estimation accuracy is comparable to the slit spectroscopy. To achieve similar accuracy for lower SNR cases, more spectral orders (than three) are needed.

To conclude, this new generation of spectral imagers offers the ability to infer spectral line parameters over an instantaneous two-dimensional FOV and with good estimation accuracy for a wide range of SNR. This is particularly useful for studying dynamic phenomena in targeted scenes.
6. REFERENCES


