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Monte Carlo Error Analysis in X-Ray Spectral Deconvolution*

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(Received

ABSTRACT

The deconvolution of spectral information from sparse x-ray data is a widely encountered problem in data analysis. An often-neglected aspect of this problem is the propagation of random error in the deconvolution process. We have developed a Monte Carlo approach that enables us to attach error bars to unfolded x-ray spectra. Our Monte Carlo error analysis has been incorporated into two specific deconvolution techniques: the first is an iterative convergent weight method; the second is a singular-value-decomposition (SVD) method. These two methods were applied to an x-ray spectral deconvolution problem having m channels of observations with n points in energy space. When m is less than n , this problem has no unique solution. We discuss the systematics of non-unique solutions and energy-dependent error bars for both methods. The Monte Carlo approach has a particular benefit in relation to the SVD method: it allows us to apply the constraint of spectral non-negativity after the SVD deconvolution rather than before. Consequently we can identify inconsistencies between different detector channels.

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INTRODUCTION

Deconvolution of an x-ray spectrum involves solving the following set of equations:

$$I_j = \int_{E_1}^{E_2} R_j(E)S(E)dE, \quad j = 1, \dots, N \quad (1)$$

Here I_j represents the measured current in detector j , $R_j(E)$ represents the energy-dependent detector response function for detector j and $S(E)$ represents the desired x-ray spectral intensity. The limits of the integral, E_1 and E_2 , span the photon-energy space of interest. Each quantity I_j has an assigned experimental random error σ_{I_j} . Our task is to determine not only the spectral intensity $S(E)$, but also energy-dependent error bars for $S(E)$.

Standard linear analysis provides the following equation for the error σ_{S_1} in the spectral intensity $S(E_1)$ at the 1 th discrete energy point E_1 :

$$\sigma_{S_1}^2 = \sum_{j=1}^N \left(\frac{\partial S(E_1)}{\partial I_j} \right)^2 \sigma_{I_j}^2 \quad (2)$$

To evaluate these terms requires a complicated analysis that is specific to the method of deconvolution used. Additionally, Eq. (2) neglects first derivative products and higher order derivatives.

To circumvent these difficulties, we have developed a form of Monte Carlo error analysis that allows us to evaluate σ_{S_1} as a function of energy. This error analysis is independent of the deconvolution method; we have used both an iterative method and a singular-value decomposition (SVD) method to perform the deconvolution.

We consider four topics: (1) calculation of random error for known detector currents using both deconvolution methods; (2) correlations or "overlap" among detectors and their effect upon the random error of the deconvolved spectrum; (3) inconsistency among correlated detector currents which might indicate the presence of systematic error; and (4) the effect of an intentionally introduced systematic error in the detector current upon the deconvolved spectrum and its error bars.

1. MONTE CARLO ANALYSIS AND METHODS

The Monte Carlo error analysis assumes that each of the N experimentally measured currents (I_j in Eq. (1)) lies at the mean of a Gaussian probability distribution whose width is set equal to the experimental error σ_{I_j} . We randomly sample from the N probability distributions to generate many "artificial" values of detector currents. In this study the number of trials or artificial current data sets was 5000. By applying a deconvolution algorithm to each of the 5000 current data sets, we obtain 5000 deconvolved spectra. A mean spectral intensity and standard deviation can be calculated from the 5000 values of spectral intensity $S(E_i)$ at each discrete point E_i in energy space. These standard deviations, σ_{S_i} , are taken to be the energy-dependent error bars for the spectrum $S(E)$. The probability density distribution of the spectral intensity is also calculated at each energy point. This gives the relative frequency of occurrence of any value of $S(E_i)$. The detailed structure of this distribution conveys much more information than a knowledge of only the mean value of $S(E_i)$ and its standard deviation.

As an illustration, the Monte Carlo error analysis was applied to a test problem in which five known (calculated) currents were generated from a 400-eV Planckian and five typical x-ray detector response functions, via

Eq. (1). Typical experimental errors were assigned to these currents. These five currents and their errors thus constituted a data set that could be analyzed in the manner just discussed. The deconvolution was performed using the SHAZAM code.¹ This deconvolution technique is iterative and requires an initial guess for the spectrum. In the deconvolution process the five experimental currents are weighted according to their assigned errors. The energy range from 0.1 to 5 keV was discretized into 200 points.

The result of the analysis is shown in Fig. 1. The solid line indicates the mean spectral intensity at each energy point. The dashed lines indicate the $\pm 1\sigma$ envelopes calculated by the Monte Carlo approach. The envelopes are energy dependent. This results from the particular form of the detector response functions and the amount they overlap in their energy coverage. The greater the overlap, the smaller the error bar in the deconvolved spectrum, because multiple measurements of a quantity reduce its random error.

Figure 2 shows a detector current "scatter plot". Each point corresponds to one of the 5000 deconvolved spectra. The coordinates of the points are the "deconvolution-calculated" currents for the indicated pair of detectors. That is, the currents result from substituting the deconvolved spectrum back into Eq. (1). The scatter occurs because the deconvolution technique does not force an exact match to the input Monte Carlo-generated "artificial" currents, which themselves have a degree of scatter due to the Gaussian distribution. A distinct elliptical form can be seen in the point distribution. Clearly certain current pairs are "preferred" and show well-defined boundaries. This correlation occurs because the detector response functions overlap significantly.

The detector correlation is quantified in Fig. 3. The original "real" experimental current and error for this detector pair is represented by the cross in the figure. Figure 3 also shows that the "covariance ellipse", calculated from the point distribution of Fig. 2, has a substantial angle of inclination and a shortening of the axes relative to the axes of the cross.² The center of the cross is quite near the center of the ellipse. This indicates a negligible amount of systematic error in the experimental currents, as expected, because these currents were known from the 400-eV Planckian spectrum. This result also serves as a check on the deconvolution procedure and the Monte Carlo error analysis.

A second method of deconvolution was also used with the Monte Carlo analysis for the 400-eV Planckian test problem. This method of deconvolution uses singular-value decomposition (SVD)^{3,4} to solve the set of matrix equations resulting from the discretization of Eq. 1. This method does not require an initial guess for the spectrum. Figure 4 shows the mean and standard deviation in the spectral intensity found using the SVD technique. The structure of this spectrum is not as smooth as that from the SHAZAM deconvolution (Fig. 1). This effect is a result of a greater dependence on the detector response functions and a minimal amount of smoothing after the SVD deconvolution. By contrast, spectral smoothing is performed after every iteration in the SHAZAM code. We consider the agreement between Figs. 1 and 4 to be reasonable, considering that the problem has no unique solution. This is because there are only 5 detectors while information is required for 200 points in energy space. The detector pair scatter plots and covariance plots for the SVD deconvolution are essentially the same as for the SHAZAM deconvolution.

II. THE EFFECT OF SYSTEMATIC ERROR

We now address briefly the question of the sensitivity of the two deconvolution techniques and the Monte Carlo analysis to a known systematic error. The systematic error was introduced by increasing one of the experimental currents for the 400-eV Planckian problem by four times the error bar. The assumed random error in the "new" current was unaltered. Specifically the old value for detector current 4 was 0.59 ± 0.07 amp while the new value was 0.85 ± 0.07 amp. Thus, detector 4 had a current inconsistent with the 400-eV Planckian spectrum. The SVD and SHAZAM deconvolutions with Monte Carlo error analysis were used to obtain deconvolved spectra. The mean spectral intensities and the $\pm 1\sigma$ envelopes from the SVD deconvolution are shown in Fig. 5. There is a clear shift in the centroid and width of the spectral structure compared to Fig. 4. This result shows the drastic effects of an undiscovered systematic error. Other effects of the systematic error are shown in Fig. 6. This figure shows the covariance ellipse of the "new" deconvolution-calculated current pairs and the new value for the experimental current pair. Comparing Fig. 3 and 6, it is clear that the distance between the centers of the ellipse and the cross has increased dramatically with the introduction of the systematic error. The SHAZAM study also showed drastic spectral changes, but the covariance plot was less affected, probably because of the dependence of SHAZAM upon an initial guess.

Another measure of the systematic error results from the use of the Monte Carlo error analysis with the SVD deconvolution. Because the SVD technique will allow negative spectral intensities if unconstrained, we apply a nonnegative spectral constraint to the solution as follows: if the deconvolved spectrum has any negative values in the energy range of

interest, we discard the solution and do not use it in the mean and standard deviation calculations. For the unperturbed current case, there were 3683 successful nonnegative deconvolutions out of 5000 trials. For the perturbed current case, simulating a systematic error, there were only 330 nonnegative deconvolutions for 5000 trials. Thus the $4\text{-}\sigma$ perturbation reduced the success rate by about a factor of ten. Further studies are underway to identify a mathematical relation between the amount of systematic error and the success rate of the SVD deconvolution.

III. CONCLUSIONS

The Monte Carlo error analysis, utilizing random sampling from a distribution based on observed currents, provides consistent and reasonable energy dependent error bars for a deconvolved spectrum. The error analysis is independent of the deconvolution method used. The effects of systematic error can be identified using the SVD deconvolution in conjunction with the Monte Carlo analysis.

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Figure Captions

Fig. 1. Mean spectral intensity (solid line) and $\pm 1\sigma$ envelopes (dashed lines) using SHAZAM deconvolution and Monte Carlo error analysis.

Fig. 2. Detector current scatter plot for detectors 4 and 5 using SHAZAM deconvolution. The plotted points represent the "deconvolution-calculated" current pair values for detectors 4 and 5.

Fig. 3. Covariance ellipse plot and "experimental" (known) current value pair for detector 4 and 5 using SHAZAM deconvolution. The ellipse represents a contour of constant probability for a detector current pair. The cross represents the "experimental" current pair and uncertainty.

Fig. 4. Mean spectral intensity (solid line) and $\pm 1\sigma$ envelopes (dashed lines) using SVD deconvolution and Monte Carlo error analysis.

Fig. 5. Mean spectral intensity (solid line) and $\pm 1\sigma$ envelopes (dashed lines) for the perturbed current case (detector 4). SVD deconvolution and Monte Carlo error analysis were used.

Fig. 6. Covariance ellipse plot and "experimental" (known) current pair for detectors 4 and 5 using the perturbed current value for detector 4.