SRON – SPEX

Differential Emission Measure (DEM) Analysis

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prepared by

R. Mewe SRON Utrecht

Contents

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1 Introduction

In many sources the X-ray spectrum is not a unique function of one single temperature (isothermal approximation with a temperature-independent emission measure), but instead is determined by a distribution in temperature across the emission region (multi-temperature approach). In the latter case the observed spectra are described in terms of a differential emission measure (DEM) distribution over the range of temperatures for which the instrument is sensitive.

By some inversion technique one can derive the DEM from the observed spectrum, using a library of theoretical spectra produced by the optically thin spectral code (and convolved with the considered instrument response).

Before we proceed we define here the differential emission measure in the following manner. The observed spectral flux $F(\lambda)$ (counts s^{-1}) measured at Earth by a given instrument at wavelength λ can be expressed as:

$$F(\lambda) = \frac{1}{4\pi d^2} \oint f(\lambda,T) n_e^2 dV = \frac{1}{4\pi d^2} \int f(\lambda,T)\varphi(T)\, dT \equiv \frac{1}{4\pi d^2} \int f(\lambda,T) T\varphi(T)\, d\ln T,$$

where $f(\lambda,T)$ is the spectral emissivity (counts cm^5 s^{-1}) for the line plus continuum emission as a function of temperature T at wavelength λ, convolved with the instrument response function; d (cm) is the distance to the source and $\varphi(T) = n_e^2 \frac{dV}{dT}$ (cm^{-3} K^{-1}) is the differential emission measure, $n_e(T)$ is the electron density (cm^{-3}) and V the plasma volume (cm^3). Note that the total emission measure is given by $EM = \int n_e^2 dV = \int T\varphi(T) d\ln T$.

The DEM is derived from the observed spectrum by deconvolving $T\varphi(T)$ from the measured spectral intensities, using the library of theoretical spectra. In the following we discuss two inversion methods.

2 Iterative Withbroe-Sylwester method

In the past we have applied for this deconvolution an iterative technique that is based on a weighting-factor method originally proposed by Withbroe (1975), modified a few years later by Sylwester, and described by Sylwester *et al.* (1980), to interpret high-resolution X-ray spectra of solar flares (Withbroe-Sylwester method).

The DEM technique was subsequently extended to broader wavelength ranges by Lemen, Mewe and Schrijver (1989) and applied to the analysis of *EXOSAT* transmission grating spectra of various late-type stars (Lemen *et al.* 1989, Schrijver *et al.* 1989). Later on (around 1992) Alkemade and Schrijver developed a software package that originally was intended to be built in SPEX for the analysis of the observed *EUVE* spectra and that contains a modified version of the original Sylwester algorithm.

In document SRON/SPEX/TRPB01 (Sections 5.3.3. and 7.1.) we give a description of this method with various examples of the results of fits on data and on simulated spectra.

However, in the mean time Schrijver and Alkemade developed the software using another inversion technique as discussed by Craig and Brown (1986) which uses a second-order regularization (smoothing). This routine has now been built in SPEX and replaces a previously used Sylwester routine. In the following we give a description of the method (see also Mewe *et al.* 1994) with a slightly different definition of the differential emission measure.

3 Inversion method of regularization

3.1 Formulation of the problem

The spectra emitted by stellar coronae are assumed to be linear combinations of isothermal plasmas: stellar coronae are optically thin, so that all temperature components are visible. The weighting function that measures the visibility of any component in the observed spectrum depends, among other things (as discussed below), on the emissivity of the plasma given temperature and density. As a consequence of the linearity of the problem, all temperatures simply add to the observed spectrum, regardless of where they occur on the disk or, in the case of binaries, on which binary component they occur. In our models we implicitly assume that all components are in thermal ionization equilibrium, thus ignoring possible transient effects, and we ignore effects associated with the plasma density.

The observed spectra are interpreted as statistical realizations of linear combinations of isothermal spectra which are calculated using our code for optically thin plasmas. We address the inversion problem of recovering the weighting function mentioned above, referred to as the "differential emission measure (DEM) distribution" $\mathbf{D} = n_e^2 dV/d\ln T$ from the observed spectrum.

3.2 The inversion problem

The method of inversion used in the present paper is described by Craig and Brown (1986) and Press *et al.* (1992). Here we present a brief summary of the method and emphasize various specific points concerning the inversion of *EUVE* spectra: Let an isothermal plasma of temperature T emit a spectrum that, when incorporating interstellar absorption, instrumental efficiencies, and instrumental smoothing, is observed as $\mathbf{f}(\lambda, \mathrm{T})$. For a composite plasma with temperatures ranging from T_0 up to T_m the net observed spectrum $\mathbf{g}$ is given by:

$$\mathbf{g}(\lambda) = \int \mathbf{f}(\lambda, \mathrm{T})\mathbf{D}(\mathrm{T})\, d\ln \mathrm{T}. \tag{1}$$

Eq. (1) constitutes a Fredholm equation of the first kind for $\mathbf{D}(\mathrm{T})$. When discretized into bins in temperature (on a logarithmic grid of temperatures $\mathrm{T_j} = \mathrm{T}_0, \cdots, \mathrm{T}_\mathrm{m}$) and wavelength (in wavelength intervals of width $\Delta\lambda$ at values $\lambda_\mathrm{i} = \lambda_0, \cdots, \lambda_\mathrm{n}$) this can be written as a vector equation:

$$\mathbf{g} = \mathbf{F} \cdot \mathbf{D} \tag{2}$$

in which $\mathbf{F}$ is a matrix composed of m columns and n rows, of which the elements are given by $\mathbf{F}_{\rm ij} = \int_{\lambda_{\rm i}}^{\lambda_{\rm i}+\Delta\lambda} \mathbf{f}(\lambda, {\rm T_j}) d\lambda \Delta \ln {\rm T} \equiv \mathbf{f}_{\rm i}({\rm T_j}) \Delta \ln {\rm T}$. Each column of $\mathbf{F}_{\rm ij}$ consists of a 'spectral' vector containing the discretized spectrum at a certain temperature. The formal least-squares solution of this problem requires an inversion of

$$\mathbf{F}^T \mathbf{F} \cdot \mathbf{D} = \mathbf{F}^T \cdot \mathbf{g} \tag{3}$$

in which $\mathbf{F}^T$ is the transpose of $\mathbf{F}$. Note that the terms $[\mathbf{F}^T \mathbf{F}]_{ij}$ are proportional to dot products $\mathbf{f}_i \cdot \mathbf{f}_j$ while the terms $[\mathbf{F}^T \mathbf{g}]_j$ are proportional to $\mathbf{f}_j \cdot \mathbf{g}$. Basically, the inversion algorithm aims at decomposing $\mathbf{g}$ into the spectral vectors $\mathbf{f}$ with the components of $\mathbf{D}$ being the multiplicative constants. This inversion process is however ill-conditioned for a Fredholm equation of the first kind. The reason is that the kernel of Eq. (1) in general smoothes the information contained in the DEM and that during the inversion process this information can not be retrieved. Therefore the inversion process is not unique. In fact, any polynomial of order $p > m$ can be made to satisfy Eq. (1). This implies that the results of inversion methods based on the iterative relaxation of an (assumed) initial DEM have to be considered with great care. In other words: the column vectors $\mathbf{f}$ which make up $\mathbf{F}$ do, in general, not constitute a orthogonal set.

Let us now consider the case that $\mathbf{g}$ represents an observed spectrum, indicated as $\widetilde{\mathbf{g}}$, which contains noise. Measurement errors can then be taken into account by defining s as the geometric mean of errors ($s^n = s_1 \cdot s_2 \ldots s_n$) and by letting $\widetilde{\mathbf{g}}_{\rm i} \rightarrow s\widetilde{\mathbf{g}}_{\rm i}/s_{\rm i}$ and $\mathbf{F}_{\rm ij} \rightarrow s\mathbf{F}_{\rm ij}/s_{\rm i}$. The solution of Eq. (3) will now be subjected to the influence of data noise which will cause artificial high-frequency oscillations in the behaviour of $\mathbf{D}$. The classical way of obtaining the solution is by minimizing the functional (generalized least squares)

$$\min \left| \mathbf{F} \cdot \mathbf{D} - \widetilde{\mathbf{g}} \right|^2 \tag{4}$$

in which one recognizes the χ^2-method. Because information concerning $\mathbf{D}$ is lost, by the action of the kernel in Eq. (1), and because no unique solution exists, it is useful to impose an additional constraint on the solution next to the classical χ^2-constraint. By assigning certain properties to the solution one limits the possible classes of solutions. Any additional constraint can formally be written as $\mathbf{R} \cdot \mathbf{D}$ which represents some functional of the DEM. A constraint which requires the DEM to be positive is in general found to be too restrictive (see Thompson, 1991). A more general class of constraints are those for which the first or second derivative of the DEM is minimized. Because derivatives of the DEM can be positive or negative it is useful to work with a quadratic constraint in the form $|\mathbf{R} \cdot \mathbf{D}|^2$. The solution of the problem now consists of minimalizing two functionals, the classical χ^2 together with $|\mathbf{R} \cdot \mathbf{D}|^2$. Each of these functionals can be regarded as a constraint to the other. Eq. (4) can then be replaced by

$$\min \left(\left| \mathbf{F} \cdot \mathbf{D} - \widetilde{\mathbf{g}} \right|^2 + \varrho \left| \mathbf{R} \cdot \mathbf{D} \right|^2 \right), \tag{5}$$

where ϱ is a Lagrangian multiplier commonly refered to as the *regularisation parameter*. The matrix form of the regularized solution is then given by

$$(\mathbf{F}^T \mathbf{F} + s^2 \, \varrho \mathbf{R}) \cdot \mathbf{D} = \mathbf{F}^T \cdot \widetilde{\mathbf{g}}, \tag{6}$$

while the mean square uncertainty of $\mathbf{D}_{\rm j}$ is given by

$$\sigma_{\rm j}^2 = s^2 [(\mathbf{F}^T \mathbf{F} + s^2 \varrho \mathbf{R})^{-1}]_{\rm jj}. \tag{7}$$

The advantage of using a quadratic minimization principle together with a quadratic constraint is that, in contrast to Eq. (3) , the left hand side of Eq. (6) is now non-degenerate so that the problem has become well-posed (see Press *et al.* 1992).

The regularization parameter ϱ ($0 \leq \varrho < \infty$) controls the degree of smoothness of the solution. This can clearly be seen in Eq. (5). The value of ϱ controls the relative weight of the χ^2-constraint with respect to the $|\mathbf{R} \cdot \mathbf{D}|^2$-constraint. In the limit $\varrho \rightarrow 0$ the χ^2-constraint becomes more important while for $\varrho \rightarrow \infty$ the DEM-constraint becomes more important. There exist both subjective and objective criteria for choosing a specific value for ϱ. Because the aim of the whole exercise is to select that specific DEM which accurately models the data, the best choice for ϱ is one which makes χ^2 comparable to the number of degrees of freedom, so for which $\chi^2_{\rm red}$ approaches unity. Note that, as a criterium for selecting ϱ, χ^2 is only used as an *a posteriori* measure of the goodness of the fit. If the model spectra contain imperfections, e.g. not all observed lines are contained within the model, then the limit $\chi^2_{red} \approx 1$ will of course not been reached.

A suitable choice for the quadratic constraint is given by $\mathbf{R} \cdot \mathbf{D} = \mathbf{D}''$ which leads to second-order regularization. With this choice one aims to select that specific DEM for which the second derivative is as smooth as possible and which is consistent with the data. If we choose as boundary conditions that $\mathbf{D}'' = 0$ at T_0 and T_m then the matrix $\mathbf{R}$ is given by

$$\mathbf{R} = \begin{pmatrix} 1 & -2 & 1 & 0 & \dots & & & & \\ -2 & 5 & -4 & 1 & 0 & \dots & & & \\ \vdots & \ddots & & & & & & & \vdots \\ \dots & 0 & 1 & -4 & 6 & -4 & 1 & 0 & \dots \\ \vdots & & & & & & & \ddots & \vdots \\ & & & \dots & 0 & 1 & -4 & 5 & -2 \\ & & & & \dots & 0 & 1 & -2 & 1 \end{pmatrix} \tag{8}$$

The structure of the matrix clearly shows the smoothing over 5 adjacent temperature intervals. If this width is smaller than the expected resolution of the process then the smoothing is likely to be insufficient. Higher order regularizations imply that more neighbouring temperature intervals become coupled. The choice for smoothing over three intervals, and hence the choice of the constraint $\mathbf{R} \cdot \mathbf{D} = \mathbf{D}''$, is not arbitrary but is based on the intrinsic properties of X-ray spectra. This is discussed below.

We stress that the above inversion method is *not* an iterative procedure. An iterative method requires an initial DEM distribution, and, depending on the details of the distribution, the iteration may not converge to the true best-fit solution, but may instead yield a solution corresponding to a local minimum in the χ^2-space (or any other measure of quality that may be used). This problem is avoided by the method of regularization.

3.3 General considerations concerning the inversion strategy

The finite width, σ_T, of the temperature intervals over which any given spectral line contributes to the observed spectrum leads to an intrinsic limit to the temperature resolution that can be achieved, regardless of the spectral resolution of the instrument. The result of the finiteness of σ_T is that intervals of formation temperatures of different spectral lines overlap. Hence, temperature information is spread out over the typical width σ_T of the temperature intervals over which the lines are strong, i.e. over the width of the formation interval for a single line which is generally roughly a factor of two in temperature ($\sigma_\mathrm{T}/\mathrm{T} \approx 2$).

The effects of a finite $\sigma_{\rm T}$ can be inferred from Eq. (3). In § 3.2. we already noted that the spectral vectors $\mathbf{f}$, which make up the columns of $\mathbf{F}$, constitute a base on which the observed spectral vector $\widetilde{\mathbf{g}}$ is projected. In the ideal case the vectors $\mathbf{f}$ constitute an orthogonal set so that the matrix $\mathbf{F}^T\mathbf{F}$ can be cast in a diagonal form, permitting a unique inversion. For a finite $\sigma_{\rm T}$, however, the matrix $\mathbf{F}^T\mathbf{F}$ maintains a diagonal shape, but the effective "width" of the diagonal band is equivalent to a temperature interval of approximately $\ln\sigma_{\rm T}/\Delta\ln{\rm T_j}$, so that a DEM consisting of a delta peak in element j ($\mathbf{D}_k = 1$ for $k = j$;$\mathbf{D}_k = 0$ for $k \neq j$) is transformed into a peak in $\mathbf{F}^T\mathbf{F}\cdot\mathbf{D}$ with a width of $\ln\sigma_{\rm T}/\Delta\ln{\rm T_j}$ elements. Similarly, an isothermal source will yield a run of $[\mathbf{F}^T\cdot{\rm g}]_{\rm j}$ with a width of $\ln\sigma_{\rm T}/\Delta\ln{\rm T_j}$ elements. Deriving $\mathbf{D}$ for an isothermal plasma from $\widetilde{\mathbf{g}}$ in the presence of noise and with a finite regularization will yield a peak only somewhat narrower than $\sigma_{\rm T}$. Significant separation of two delta functions is possible only if the spacing between the peaks is at least about $2\sigma_{\rm T}$.

If the spectral resolution of the instrument is such that spectral lines formed at different temperatures cannot be separated, an even more troublesome problem develops: if information from significantly different temperatures is contained within the same wavelength interval, observational noise allows the spreading of information from one temperature to another. Imposing smoothing constraints therefore contaminates the $\mathbf{D}$ at very different temperatures. With worsening resolution, the off-diagonal elements of $\mathbf{F}^T\mathbf{F}$ become stronger and stronger, relative to the diagonal elements, thus increasing the interdependence of the rows and columns, and making the problem more and more ill-posed.

It will be clear from the above considerations that both the continuum emission and the instrumental background noise cause some degree of crosstalk of information over the entire temperature interval studied, resulting in a broad "wing" to the diagonal of $\mathbf{F}^T\mathbf{F}$. We note that despite the problems arising from the presence of a continuum it is important to fit both lines and continuum simultaneously given the fact that we found that the line-to-continuum ratio plays an important rôle in *EUVE* spectra.

3.4 Optimal binning for a DEM inversion.

In view of the discussion in § 3.3., we argue that contamination of $\mathbf{D}$ over temperature ranges exceeding the formation width of individual lines is limited if bins containing only continuum information and bins containing lines formed at significantly different temperatures, and bins with low S/N ratios are given a low weight. In the *EUVE* spectra these conditions are largely fulfilled automatically if the spectra are weighted with the observational uncertainties, as discussed above: lines formed at different temperatures are generally well separated, and the continuum bins have low count rates, and thus relatively large uncertainties, so that the error weighting automatically reduces the influence of these bins on the result of the inversion procedure. Because the temperature resolution is limited to approximately $\ln\sigma_{\rm T}$, the spacing of the temperatures $\Delta\ln{\rm T}$ needs not be chosen much smaller than that. In fact, the regularization matrix $\mathbf{R}$ should be chosen in a way to smooth over intervals of about the width $\ln\sigma_{\rm T}$, because otherwise unrealistic features may be introduced. Combination of these two statements results in the suggestion that the temperature resolution for $\mathbf{D}$ should be set at about $\frac{1}{2}\ln\sigma_{\rm T}$. Since in realistic situations $\sigma_{\rm T}/{\rm T} \approx 2$, logarithmic temperature intervals of $\log(\Delta\log({\rm T})) \approx 0.15$ suffice, but we use a slightly finer grid. In the analysis we use a range of temperatures from 3 10^4 K up to 10^8 K divided in 36 logarithmically spaced temperature values (i.e. $\Delta\log({\rm T}) \simeq 0.1$). The choice of the lower temperature boundary is determined by the presence of strong He II lines which form below $\sim 10^5$ K. Omitting this temperature range leads to artificially

bad χ^2. Solving Eq. (6) requires the inversion of $N \times N$ matrices if we use a temperature grid of N points. The choice of $\mathbf{R}$ (Eq. (8)) implies that information does not propagate over temperature intervals larger then a typical line formation width $\sigma_{\rm T}$.

The wavelength binning of the spectra needs not be better than slightly below the instrumental resolution σ_λ. Hence, for a wavelength interval of λ_0 to $\lambda_{\rm n}$ a total of about $(\lambda_{\rm n} - \lambda_0)/(\langle\sigma_\lambda\rangle/2)$ is sufficient, so that one may choose a binning corresponding to about half the spectral resolution.

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