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New Elements of Sherpa, CIAO's Modeling and Fitting Tool

P. E. Freeman, S. Doe, A. Siemiginowska

Harvard-Smithsonian Center for Astrophysics MS-81, 60 Garden Street, Cambridge, MA 02138

Abstract. We describe enhancements made to *Sherpa* for the CIAO 2.0 release, concentrating upon those that enable a user to: (1) analyze *Chandra* X-ray Observatory grating data with wavelength- or energy-space models; (2) simultaneously fit background and source datasets; and (3) estimate and visualize confidence intervals and regions. We also list enhancements that we plan to make to *Sherpa* for future CIAO releases.

1. Introduction

Sherpa is the modeling and fitting tool of the *Chandra* Interactive Analysis of Observations (CIAO) software package (Doe et al. 1998 and references therein). We have developed it with the primary goal that a user should be able to take full advantage of *Chandra*'s unprecedented observational capabilities and be able to analyze data in up to four dimensions (energy E or wavelength λ, time t, and spatial location $[x, y]$) with a wide variety of models, optimization methods, and fit statistics. The enhancements that we have made to *Sherpa* for the CIAO 2.0 release, described below, represent major steps towards this goal.

2. Enhancements to Sherpa

2.1. Grating Analysis

Data Analysis in Wavelength and Energy Space. *Chandra* grating data are most naturally analyzed in wavelength space, while *XSPEC* line models such as `xsraymond` are defined in energy space.[1] *Sherpa* now allows one to define models in either space, while using either grating Ancillary Response Files (gARFs) or Response Matrix Files (gRMFs) or both. The `ANALYSIS` command allows one to switch between spaces.[2] One can also now apply filters defined in wavelength or energy space to single datasets, groups of datasets, or to `allsets`. See Figure 1.

[1]Models in the *XSPEC* v.10 library are available to users of CIAO 2.0, while the v.11 library will be available starting with CIAO 2.1.

[2]The reader will find more information about `ANALYSIS`, as well as all other *Sherpa* commands, at `http://asc.harvard.edu/ciao/documents_manuals.html`.

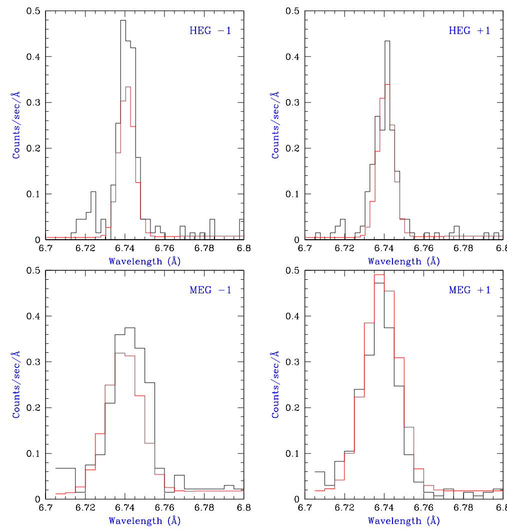

Figure 1. Best-fit of a normalized Gaussian function to an emission line observed in four first-order HEG and MEG *Chandra* grating spectra of Capella. The amplitude, full-width at half-maximum, and position values are linked between datasets. The `identify` function of *GUIDE* indicates that line is most likely due to the Si XIII 2→1 transition at 6.7403 Å.

Data Analysis with Two Background Spectra. Standard processing of *Chandra* grating data includes the extraction of background spectra, dubbed "up" and "down," from either side of the source extraction region. One can either fit both spectra simultaneously with the source spectrum (see below), or `SUBTRACT` both from the source spectrum.

The Grating User Interactive Data Extension (GUIDE). This S-lang-based extension to *Sherpa* assists the fitting of atomic lines and differential emission measure (DEM). For more information, see Doe, Noble, & Smith (2001) and `http://asc.harvard.edu/ciao/download/doc/guide_doc.ps`.

Saving Analysis Results. One can save and restore a *Sherpa* session using a Model Descriptor List (MDL) file, which records information about input datasets, and filter and model definitions. One example of its usefulness is in DEM fitting, where the input data are MDL-stored line fluxes and flux errors.[3]

2.2. Simultaneous Analysis of Background and Source Data

Previous versions of *Sherpa* allowed the user to input background data with the commands `BACK` or `READ BACK`, but these data could only be subtracted from

[3] Flux errors are easily estimated for three *Sherpa* models for which the amplitude is equal to the flux: the normalized Gaussian (`ngauss`); the delta function (`delta`); and the Lorentzian (`lorentz`).

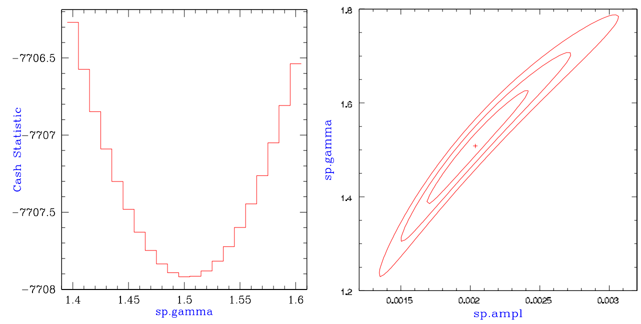

Figure 2. Examples of parameter space visualization. *Left:* A plot showing the Cash statistic as a function of power-law slope, generated using `INTERVAL-PROJECTION`. *Right:* contour plot showing 1, 2, and 3σ confidence regions for the power-law amplitude and slope, generated using `REGION-PROJECTION`. The central cross indicates the best-fit point.

the source data. *Sherpa* now allows the simultaneous analysis of one (or two) background dataset(s) for every source dataset that is read in. A background model is fit directly to the background data, and is also extrapolated to the source region, where it is added to the source model before convolution. Rescaling for different extraction region sizes is done using the values of the `BACKSCAL` keyword, set in the header of the PHA files containing source and background data, using the commands `SETDATA` and `SETBACK`.

2.3. Estimation of Confidence Intervals and Regions

Sherpa contains many new methods that one can use to estimate confidence intervals or visualize confidence regions for best-fit model parameters. Note that these methods are strictly valid, i.e., provide 1σ confidence intervals that actually contain 68.3% of the integrated probability, when (1) the χ^2 or $\log\mathcal{L}$ (log-likelihood) surface in parameter space is approximately shaped like a multi-dimensional paraboloid, and (2) the best-fit point is sufficiently far from parameter space boundaries.

Uncertainty. The confidence interval is determined for each parameter in turn by varying its value while holding the values of all other parameters at their best-fit values. While fast, `UNCERTAINTY` will underestimate a parameter's interval if it is correlated with other parameters. One can visualize spaces with `INTERVAL-UNCERTAINTY` and `REGION-UNCERTAINTY`.

Projection. The confidence interval is determined for each parameter in turn while allowing the values of all other parameters to float to new best-fit values. One can visualize spaces with `INTERVAL-PROJECTION` and `REGION-PROJECTION` (see Figure 2).

Covariance. The confidence interval for each parameter is determined using the diagonal terms of the covariance matrix. While fast, it cannot be used to visualize parameter spaces.

2.4. Other Enhancements

Below we list other enhancements to *Sherpa* made for the CIAO 2.0 release.

- We have extensively retooled the algorithms for the optimization methods `POWELL`, `SIMPLEX`, and `LEVENBERG-MARQUARDT` to make them more robust.
- The parameter value guessing algorithm now takes into account the exposure time and ARF if PHA spectral data are input.
- One can use ARFs and RMFs with different photon-space binning.
- One can simulate one-dimensional spectra with `FAKEIT`.
- One can define two-dimensional spatial models in either image coordinates or in the World Coordinate System (WCS).
- New models other than `ngauss` and `delta` include a broken power law (`bpl`), one- and two-dimensional constants (`const` and `const2d`), a two-dimensional delta function (`delta2d`), a phenomenological photoionization edge model (`edge`), and a line broadening model (`linebroad`).
- One can set preferences in a `.sherparc` file in the home directory.

3. Selected Future Enhancements to Sherpa

Spectral Fitting. *Sherpa* does not yet treat photon "pile-up," which can markedly affect the fitting of energy spectra of strong sources observed by either *Chandra* or *XMM*. Another *Chandra*-specific enhancement would be the ability to convolve data with analytic functions specified in Fits Embedded Function (FEF) files (Rots et al. 2001), rather than a response matrix, which could markedly decrease the time needed to analyze grating spectra.

Spatial Analysis. Currently, *Sherpa* cannot apply exposure maps in spatial analysis, nor can it calculate the fluxes in two dimensions. Also, the current *Sherpa* requirement that a one-to-one mapping exist between each background bin and source bin must be waived so that, e.g., one can define differently sized source and background regions in an image.

Statistics. Enhancements to be made include adding model comparison tests, correlation analysis and non-parametric fitting, and support for Bayesian analyses (e.g., specification of the prior and credible interval/region estimation).

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