Fitting and Modeling of AXAF Data with the ASC Fitting Application

S. Doe, M. Ljungberg, A. Siemiginowska and W. Joye

AXAF Science Center, MS 81, Smithsonian Astrophysical Observatory, 60 Garden Street, Cambridge, MA 02138 USA

Abstract. The AXAF mission will provide X-ray data with unprecedented spatial and spectral resolution. Because of the high quality of these data, the AXAF Science Center will provide a new data analysis system—INCLUDING a new fitting application. Our intent is to enable users to do fitting that is too awkward with, or beyond, the scope of existing astronomical fitting software. Our main goals are: 1) to take advantage of the full capabilities of the AXAF, we intend to provide a more sophisticated modeling capability (i.e., models that are \( f(x, y, E, t) \)), models to simulate the response of AXAF instruments, and models that enable “joint-mode” fitting, i.e., combined spatial-spectral or spectral-temporal fitting); and 2) to provide users with a wide variety of models, optimization methods, and fit statistics. In this paper, we discuss the use of an object-oriented approach in our implementation, the current features of the fitting application, and the features scheduled to be added in the coming year of development. Current features include: an interactive, command-line interface; a modeling language, which allows users to build models from arithmetic combinations of base functions; a suite of optimization and fit statistics; the ability to perform fits to multiple data sets simultaneously; and, an interface with SM and SAOting to plot or image data, models, and/or residuals from a fit. We currently provide a modeling capability in one or two dimensions, and have recently made an effort to perform spectral fitting in a manner similar to XSPEC. We also allow users to dynamically link the fitting application to their own algorithms. Our goals for the coming year include incorporating the XSPEC model library as a subset of models available in the application, enabling “joint-mode” analysis and adding support for new algorithms.

1. Introduction

The AXAF is NASA’s “Advanced X-ray Astrophysics Facility,” scheduled for launch on 27 August 1998. The AXAF Science Center Data Systems will provide the astronomical community with software to reduce and analyze AXAF data. In particular, our team is working on a fitting and modeling application suitable for analysis of AXAF data. We have two main design goals: to provide modeling in up to 4 dimensions, for functions truly \( f(E, x, y, t) \); and, to package together...
a wider variety of optimization algorithms and fit statistics. Meeting these goals will enable users to take advantage of the quality of AXAF data.

2. Design of the Fitting Application

Figure 1 shows the main fitting process that occurs within the application. The data are modeled by some function $F(\vec{X}, \vec{P})$, where $\vec{X}$ is the data space and $\vec{P}$ is the vector of model parameters. A fit statistic is then calculated by comparing the data to the predicted data calculated with the model. The fit statistic is used by the optimization algorithm to determine the next $\vec{P}$ to try; the application iterates through this process until the convergence criteria are reached, at which point $\vec{P}$ contains the best fit parameters.

We have taken an object–oriented approach to the design of the fitting application. Figure 2 shows an example; these are the classes associated with the “Search Parameter Space” box shown in the previous figure. Since the design for the classes associated with the other two boxes is substantially the same, we show here only the “Method” class.
We provide a number of different optimization algorithms (e.g., the simplex method, Powell minimization, grid search, etc.); each of these are contained in their own separate derived class as shown in Figure 2. All of these classes inherit from the base “Method” class, which contains information all the derived classes use. This structure has made it particularly easy for us to “plug-in” new algorithms as they are requested by our scientists. There is also a class associated with the Method class called the “MethodParam” class; this class contains the convergence criteria used by the various optimization algorithms.

Thus, we have three types of base classes to manage—the Method, Model and Statistic classes. (A “model” is composed of an arithmetic combination of functions $f(X, P)$ derived from the Model classes; the fit statistics of the Statistic classes are used to compare the data with the “predicted data” generated by models.) Figure 3 shows the managers we use to keep track of the algorithms and models currently in use. The Method and Statistic managers need merely to point at the algorithm currently in use; the Model Manager, on the other hand, needs to construct the model by evaluating three model stacks, the source, background, and instrument model stacks, and then combining them appropriately (i.e., the background model is added to the source model, and the result is convolved with an instrument model). The source model alone may be used, if no background or instrument models have been defined.

3. Current Implementation

We have implemented a version of the fitting application which is currently undergoing alpha testing at the ASC. This version has capabilities which include the following:

- Command-line interface
  - Command completion, history, vi, emacs keymaps, escape to shell.
  - Execute scripts, create logs.
• Multiple data sets
  —E.g., fit data from different missions to the same model.
• Modeling in 1 and 2 dimensions
• Filtering of data in memory
• Modeling “mini-language”
  —Build model out of arithmetic combination of functions.
• Interaction with SAOtsng, GNUPLOT, SM
• Selected XSPEC compatibility
• Dynamic linking to user algorithms
  This version will serve as the foundation of the flight version.

4. Continuing Development
The first release of ASC software is scheduled for June 1998. For the June release, we must add the following capabilities to the fitting application:

• Implementation of “joint-mode” analysis
• Modeling in up to 4 dimensions for functions truly \( f(E, x, y, t) \)
• Additional algorithms and statistical approaches
• Interface with ASC Data Model
• Support for X-ray gratings on AXAF
• Support for external AXAF simulators
• GUI

Adding this functionality to the fitting application will provide AXAF users with a powerful tool for the analysis of AXAF data.

Acknowledgments. This project is supported by NASA contract NAS8-39073 (ASC). We would like to thank Mark Birkinshaw for making his OPTIM library available at the ASC.

References
Birkinshaw, M., 1995, CfA internal memo