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The ASC Fitting Environment

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Abstract. Fitting models to data will be a crucial part of both the calibration of the AXAF instruments and the scientific analysis of AXAF data. The ASC Fitting Environment will provide a suite of fitting tools for the analysis of AXAF and AXAF-related data. The environment will incorporate and/or support current software packages (e.g., PROS, XSPEC) that provide tasks for fitting physical models to astrophysical data. In addition, the ASC Fitting Environment will offer a selection of techniques for searching parameter space (e.g., simple grid search, simplex downhill, Monte Carlo, and Powell methods), a number of fit statistics for evaluating goodness of fit (e.g., χ^2 and Cash statistics), and a variety of physical, analytical, and instrument specific models. The ASC Fitting Environment will make use of the ASC Data Model; this will allow the code to handle data in a variety of formats (e.g., FITS, QPOE), and to more easily perform fits to "stacks" of data files. In this paper, we present the requirements of the ASC Fitting Environment, as well as a high-level design of the environment.

1. Introduction

The Advanced X-ray Astrophysics Facility (AXAF) Science Center (ASC) will provide and support software for the AXAF mission. This software will be used for the calibration of AXAF instruments at the X-ray Calibration Facility (XRCF), for flight operations, and for the analysis of AXAF data. Fitting models to data will be a crucial part of both the calibration process and the analysis of astronomy data. The ASC Fitting Environment will offer users a variety of fitting methods. Release 1 of the Fitting Environment is to be used at XRCF, while Release 3 is the flight version. We present the requirements of the Release 1 Fitting Environment, as well as a preliminary design.

2. Why an ASC Fitting Environment?

We do not propose to write a completely new fitting package, but rather to adapt off-the-shelf software to our needs. Nevertheless, since other fitting packages do exist, it is legitimate to ask why the ASC should go to the trouble of providing its own fitting package. Our reasons for doing so include:

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- We will support multidimensional fitting (i.e., fits to models of arbitrary data dimensions, not just energy and position).
- Because of the extensive calibrations to be carried out at XRCF, source models and instrument models need to be treated on an equal basis, allowing fitting of data or of calibration parameters.
- We will separate the choice of the optimization scheme and the fit statistic, to provide users with a number of different approaches to fitting.
- The Environment will take advantage of the ASC Data Model (Van Stone, Conroy, & McDowell 1996) to perform fits to ASC "stacks" of data files, as well as to data within one file. In the context of the Data Model, an ASC "stack" is a table containing references to other data files.

XSPEC (Arnaud 1996) has become the standard for X-ray spectral fitting, and we are working with the Goddard Space Flight Center to ensure that XSPEC is integrated into the Release 3 Fitting Environment.

3. Requirements

The Release 1 version of the Fitting Environment is required to support the following features:

- ASC users will be fitting data to models of various instruments as well as to models of astrophysical sources. Therefore, the Fitting Environment must support a wide range of models. For Release 1, these will include analytical models (polynomial, Gaussian, Lorentzian, power law, and other common functions), user defined models (which are algebraic combinations of these analytical models), and AXAF Simulator models. These latter are models of the mirror, gratings, filters, and instrument responses, to be calibrated at XRCF.
- To support the user defined and AXAF Simulator models, we will provide a modeling "mini-language" which will allow users to define algebraic combinations of the analytic models, or models which are pipelines composed of various AXAF Simulator models.
- We will provide the χ^2 and Cash (1979) statistics as measures of the fit statistic during fitting and of the "goodness-of-fit" after fitting.
- We will provide the following parameter space search strategies: grid search, downhill simplex, Powell, Monte Carlo, and simulated annealing.
- The Fitting Environment will make use of the ASC Data Model.

4. Design

Figures 1 and 2 show a preliminary, high-level design of the Fitting Environment. Figure 1 shows the modules the user interacts with directly. Figure 2 shows the

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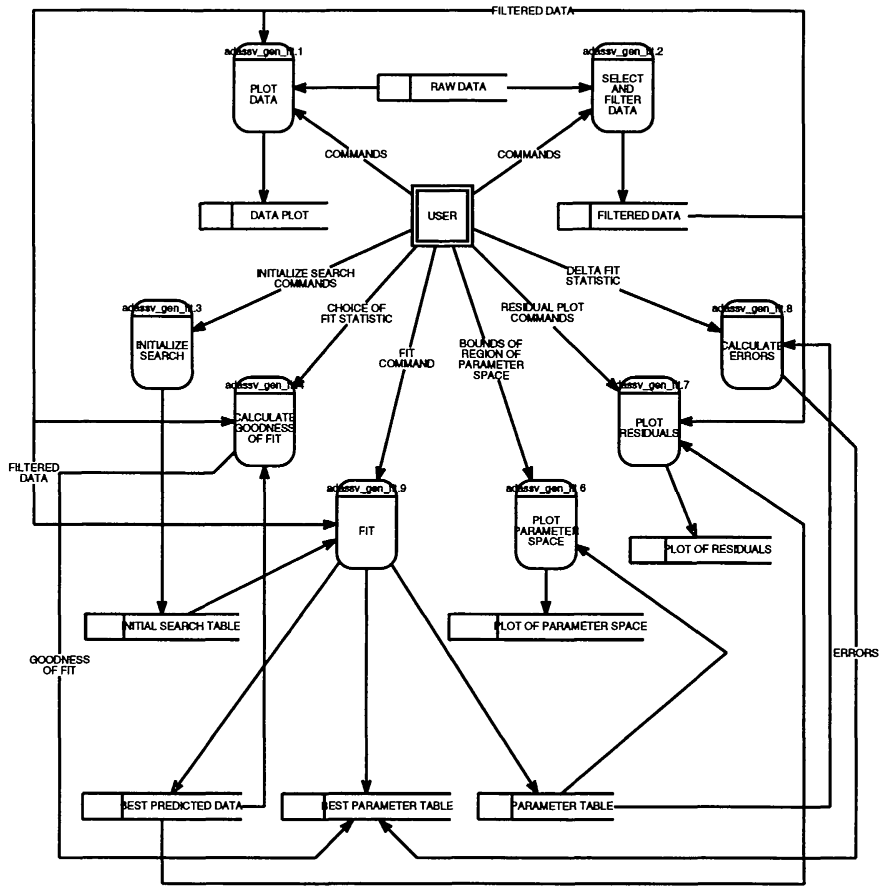

Figure 1. The ASC Fitting Environment.

steps carried out by the "FIT" module, which is responsible for finding the best parameters for a given model. As shown in Figure 1, tasks associated with fitting are:

1. The user first selects good data from the raw data, and creates a new, filtered data set upon which the fit is actually performed. The user may also plot or image the data to aid in this selection.

2. The search methods to be used must also be defined before fitting. The user constructs a table containing this information, which includes: the type of model, the number of model parameters, the initial values and ranges of the parameters, the type of search, the convergence tolerance for the search, the maximum number of iterations, and the type of fit statistic. This table gets passed to the "FIT" module, which performs the search through parameter space.

3. After fitting, the user may go on to calculate the "goodness-of-fit" for a parameterized model, calculate the errors associated with a given set of parameters, plot the residuals, and/or plot a region of parameter space.

The "FIT" module has three major components, the Model Generator, the Fit Statistic Calculator, and the Parameter Searcher. This module iterates

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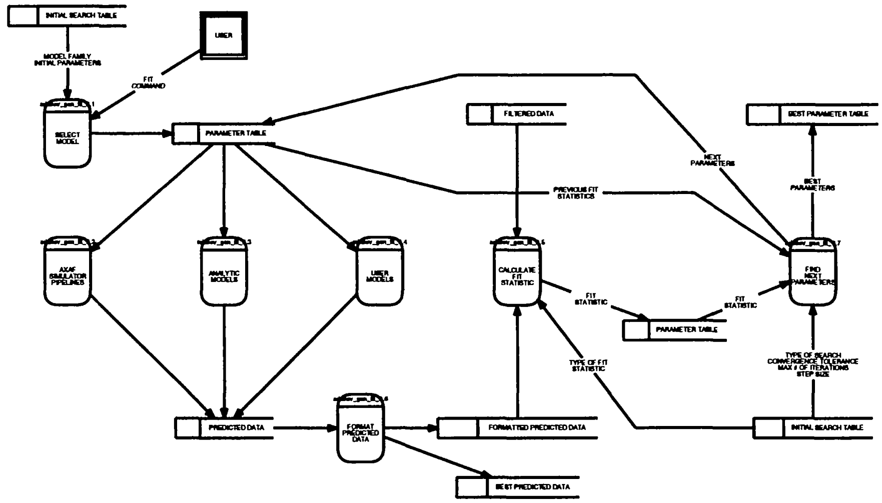

Figure 2. The "FIT" module.

through these three steps until either the best parameters have been found or the maximum number of iterations has been reached. Figure 2 shows these components.

1. The Model Generator calculates predicted data, given a parameterized model. Current values for parameters are read from the parameter table. When the best parameters have been found, the Model Generator also calculates the best predicted data, which are saved.

2. The Fit Statistic Calculator compares predicted data with the actual data, and calculates the fit statistic. This statistic is then appended to the parameter table.

3. The Parameter Searcher reads the current set of parameters from the parameter table, and finds the next set of parameters, which is written to the parameter table. If convergence has occurred, this module also finds the best fit parameters in the table, puts them into the best parameter table, passes this table to the Model Generator, and passes control back to the user.

The goal of this design is to give the user a wider range of options for fitting, and more control over the methods used to obtain a good fit.

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References

Arnaud, K. A. 1996, this volume

Cash, W. 1979, ApJ, 228, 939

Van Stone, D., Conroy, M., & McDowell, J. 1996, this volume

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