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Fitting and Modeling in the ASC Data Analysis Environment

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Abstract. As part of the AXAF Science Center (ASC) Data Analysis Environment, we will provide to the astronomical community a Fitting Application. We present a design of the application in this paper. Our design goal is to give the user the flexibility to use a variety of optimization techniques (Levenberg-Marquardt, maximum entropy, Monte Carlo, Powell, downhill simplex, CERN-Minuit, and simulated annealing) and fit statistics (χ^2, Cash, variance, and maximum likelihood); our modular design allows the user easily to add their own optimization techniques and/or fit statistics. We also present a comparison of the optimization techniques to be provided by the Application. The high spatial and spectral resolutions that will be obtained with AXAF instruments require a sophisticated data modeling capability. We will provide not only a suite of astronomical spatial and spectral source models, but also the capability of combining these models into source models of up to four data dimensions (i.e., into source functions $f(E, x, y, t)$). We will also provide tools to create instrument response models appropriate for each observation.

1. Introduction

Fitting models to data is a vital part of the analysis of astronomical data. As part of the ASC Data Analysis Environment, we have designed a Fitting Application. Although other fitting packages (e.g., XSPEC; see Arnaud 1996) exist, the high resolution and sensitivity of AXAF data present new challenges to the modeling and fitting of data; fitting models of the form $f(E, x, y, t)$ is a requirement for our software, and so we have been compelled to design our own Fitting Application. This paper presents a design of the flight version (Release 3) of our Fitting Application. We also discuss a preliminary test of the performance of the X-Ray Calibration Facility (XRCF), Release 1 version of our fitting software (Doe, Conroy, & McDowell 1996).

2. Design of the Fitting Application

The design of our Fitting Application is shown in Figure 1. The Application is controlled through a GUI, the Fit Monitor/Navigator. (The modules and tools discussed below may also be run from outside, without invoking the Navigator.) As a Monitor, it monitors the progress of the Fitting Engine through parameter

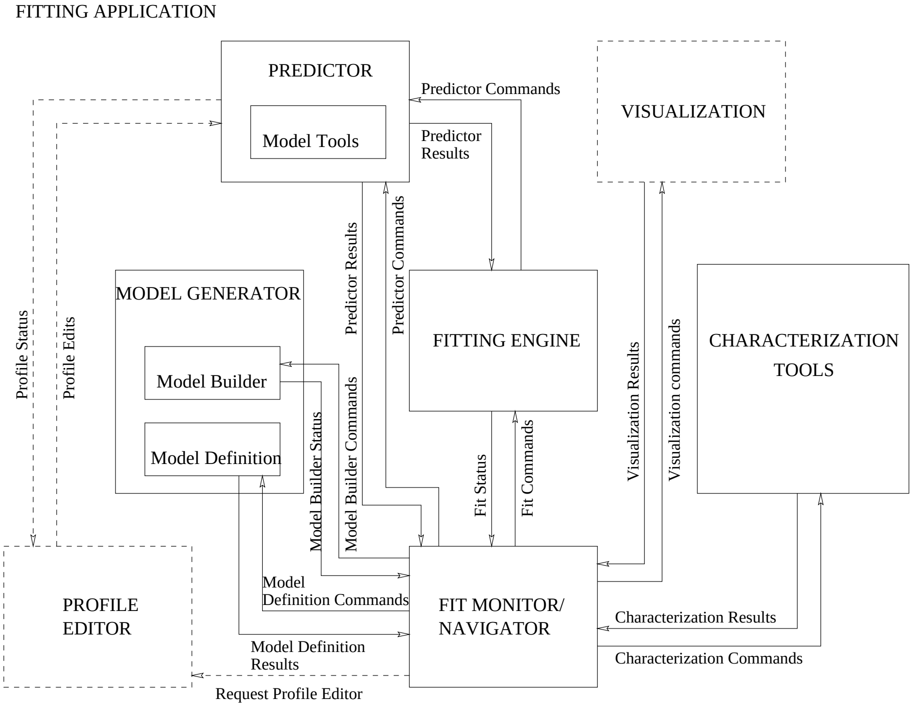

Figure 1. The Fitting Application.

space, and can halt the engine when necessary. As a Navigator, it allows the user to invoke the following utilities:

- **Fitting Engine.** This is the main component, responsible for searching parameter space. Given data, a parameterized model, and some convergence criteria, the Engine calculates predicted data values, compares them to the observed data, and searches parameter space for the parameters that yield a "best fit." The history of the search is recorded in a history file; the "best predicted data" are also calculated with the best-fit parameters. The Engine supports a variety of fit optimization algorithms, fit statistics, and convergence criteria.

- **Model Generator and Predictor.** The Model Generator has two functions. The Generator allows the user to *define* a model, by combining simpler models according to the rules imposed by the modeling language, and by setting the parameters of the model. The Generator also allows the user to *build* a model, by parsing the modeling language expression and storing the result in a format used by the Predictor. The Predictor may then take a model built by the Model Generator, and *calculate* predicted data over some data (sub)space. This may involve calls to pre-defined functions (e.g., a Gaussian or a power-law), or the execution of a series of external programs, which have been defined in a profile built with the Profile Editor.

- **Profile Editor.** With the Profile Editor, a *profile*, listing a number of programs, and their order of execution, may be built. Once such a profile has been built, it may be sent directly to the Predictor, which will execute the programs listed in the profile and store the results in a file. Data from that file may then be sent to Fitting Engine.

- **Characterization Tools.** These tools may be used to characterize a fit after a fit has been performed. Characterizing a fit may include calculating a "goodness-of-fit," performing statistical tests, calculating residuals, or determining some confidence ranges associated with the best-fit parameters.

- **Visualization.** Finally, the user may examine the results and plot the observed data, the "best-fit" predicted data, the residuals, and results from other statistical tests, in up to three dimensions. Since the search through parameter space is saved in the history file, it is also possible to plot regions of parameter space.

3. Modeling Requirements

The Fitting Application is required to support the following modeling features:

- **Empirical Models.** These models are analytical, empirical functions (e.g., polynomial, Gaussian, Lorentzian, power-law, etc.), which are not folded through instrument response models.

- **Astronomical Source Models.** These models include a variety of spatial, spectral, and temporal models of astronomical X-ray sources. Spectral models from the XSPEC package will also be available. However, the user may combine spatial, spectral, and temporal models into models capable of modeling a data space of up to four dimensions (e.g., $f(E, x, y, t)$).

- **AXAF Instrument Response Models.** Astronomical source models may be folded through AXAF instrument and mirror response models. From the instrument responses provided, a response model appropriate for a given AXAF observation may be generated. Response models appropriate for other missions (e.g., *Einstein*, *ROSAT*) may also be used.

- **Modeling Language.** Due to the high spatial and spectral resolutions of the AXAF instruments, it is highly desirable to be able to, e.g., combine models in "joint" spatial-spectral modes, which requires a modeling language sophisticated enough to permit users to build such "joint" models.

4. Comparison of Optimization Algorithms

We have implemented a Release 1 (XRCF) version of the Fitting Engine; this implementation includes the optimization algorithms listed in the table below. The implementation of the Levenberg-Marquardt algorithm is that contained in Numerical Recipes (1992); for the other algorithms, we have used the OPTIM library (Birkinshaw 1995). In this table, we present the execution time of the Engine, relative to the execution time of the Engine when the simplex algorithm has been selected. (At present, we are exploring ways to optimize the implementation of these algorithms, particularly the Powell and Levenberg-Marquardt routines.) In each run of the Engine, a 2-D Gaussian was fit to an array of 900 data points. We also present the number of lines of code for the implementation of each algorithm.

Table 1. Comparison of Optimization Algorithms.

Algorithm	Execution Time [a]	SLOCs [b]
grid search	1.6	233
grid search + Powell	2176.0	1058
Levenberg-Marquardt	3.0	332
Monte Carlo	2.7	163
Monte Carlo + Powell	477.0	977
Powell	13.3	814
simulated annealing (1)	249.6	259
simulated annealing (2)	389.4	265
simulated annealing (1) + Powell	272.4	1073
simulated annealing (2) + Powell	202.2	1079
simplex	1.0	368

[a] Relative to execution time for simplex.

[b] Source lines of code.

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