# Bayesian Analysis Users Guide
# Release 4.00, Manual Version 1

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# Chapter 1

# An Overview Of The Bayesian Analysis Software

The Bayesian Analysis Software developed at Washington University is a client/server based software package that analyzes common problems in the sciences using Bayesian Probability theory. The Software is a client/server software package consisting of three distinct sets of software: The Server software, the Client software and the Installation software. The Server software actually runs the Bayesian analysis. The Client software is an interface that functions as a buffer between the user and the server software. Finally, there is an Installation procedure that downloads and installs software.

The software is loosely divided into a series of programs which we refer to as packages. Each package addresses a specific kind of problem. For example, the exponential package estimates the parameters associated with exponential models. All of the calculations presented in this manual use Bayesian probability [1, 35] theory to estimate the parameters or to perform model selection. For those unfamiliar with Bayesian Probability theory Chapter 4 contains a tutorial, and there are a number of excellent tutorials [30, 39, 3, 11] and books [32, 58, 60, 55, 31] in the literature. Most but not all of the packages described in this manual use Markov chain Monte Carlo to approximate the Bayesian posterior probabilities. For those unfamiliar with Markov chain see [23, 44] and Section B gives a description of how the various packages implement the Markov chain Monte Carlo calculations.

## 1.1 The Server Software

Before we describe the interface, we briefly describe the server software and how the client software interfaces to it. The server, the machine that actually runs the Bayesian Analysis, can be any multi-core LinuxPC, either 32 or 64, bit running GNU/Linux (CintOS 4.7 or higher) or a Sun system running Solaris 9 or 10. When the software is installed on the server, the installation procedure downloads the latest version of the software from Washington University and installs it on the server, see Chapter 2 for instructions on how to install the software. The server software consists of three parts: a web server, a set of scripts that are used by the web server, and the programs the implement the Bayesian probability theory calculations. The web server handles the communications between the client and the server applications. The clients send requests to the servers and the servers use a set of scripts to handle these requests. These scripts do things as simple as listing the process currently running on the server; to things as complicated as unpacking an analysis and then running the appropriate software. In the following Chapters we will describe each of these software packages.

The server software contains the programs that run the Bayesian analysis packages, while the Client Interface allows one too easily access these programs. Here is a list of the packages with a brief description of each. The Client Interface Chapter, Chapter 3, contains a more extensive description of the packages, and the later Chapters in this manual contain detail information about each package.

- The Exponential package estimates the decay rate constants and amplitudes of signals known to be decaying exponentially.
- The Unknown Exponential package estimates the decay rate constants and amplitudes of signals known to be decaying exponentially when the number of exponential components are unknown.
- The Inversion Recovery package is a special type of exponential analysis that is very common in NMR. In this problem the NMR signal starts at a negative value and decays to a positive value.
- The Diffusion Tensor package analyzes NMR diffusion measurements using one, two or three diffusion tensor models with or without a constant.
- The Enter Ascii Model package allows the user to define a model and then use Bayesian Probability theory to analyze data using that model.
- The Enter Ascii Model Selection package utilizes the models generated for Enter Ascii to do model selection.
- The Test Ascii Model model package supports the other packages that use Ascii Models by giving the user a means of testing models.
- The Magnetization Transfer (two sites) package solves the Block-McConnell equations to obtain the exchange rate constants for two site magnetization exchange.
- The Magnetization Transfer Kinetics package is a magnetization transfer package that solves the Block-McConnell equations at multiple temperatures and concentrations to derive the entropy and enthalpies of the the exchange process.
- The Big Magnetization Transfer package solves the magnetization transfer problem when one of the sites can be considered infinite compared to the other.
- The Bayes Analyze package is a time domain frequency estimation package that is fully capable of determining the number of resonances in an FID and estimating the resonance parameters.
- The Big Peak/Little Peak package analyzes time domain FID data in which there is a single big peak that may be many orders of magnitude larger in intensity (the big peak) than the metabolic peaks (the little peaks) of interest.

- The Find Resonances package analyzes NMR FID data looking for resonances. The program is a model selection program that is attempting to determine the number of resonances in the data and estimate the parameters associated with those resonances.

- The Metabolite package analyzes FID data from a number of known samples, for example a C13 FID of Glutamate. The intensity of the Glutamate resonances are related to each other through a metabolic model. This model can be very simple or very complex. Metabolic models can be added to the library of models, but there are no facilities for building these models within the interface.

- The Behrens-Fisher package solves the classical medical testing problem: given two experiments that consist of repeated measurements of the same quantity where in the second measurement one has change some experiential parameter determine if the experiments are the same or if they differ.

- The Errors in Variables package solves the problem of straight-line fitting when there are errors in both the measured data and in the measured time, or abscissa value. The implementation in this package allows the user to set the order of the polynomial to be fit, so its a little more general that just straight-line fitting.

- The Polynomial Models package fits polynomials of either a given or an unknown order to the input data. When the unknown model is selected the programs that implement the calculation compute the posterior probability for the order of the polynomial needed to fit the data down to the noise.

- The Maximum Entropy Histograms density estimation package is a ASCII package that takes as its input a sample drawn from an unknown density function. It then computes the posterior probability for the number of nontrivial moments in the data, i.e., the number of Lagrange multipliers need by the Maximum Entropy density function. Its output is the estimated density function with error bars on the estimated density function.

- The Binned Histogram package estimates a binned density function with error bars. In the near future we will be enhancing this package to perform model selection. That is to say the binned histogram package will automatically determine both the number of bins and smoothing need to describe the density function.

- The Linear Phasing package produces linearly phased images. In NMR the complex image data have phases that vary across the image in a linear fashion. These linear phases are present because of the gradients that are used to generate an MR image. The linear phasing package estimates the value of the zero and first order phases in the phase encode and readout domains and then unwraps this phase so that the image can be displayed in absorption mode.

- The Non-Linear phasing package phases images that have phases that are varying in a Non-Linear fashion. In this package the phases are estimated on a pixel by pixel basis and the estimated phase is used to generate an absorption mode image.

- The Image Pixels package loads a one of the predefined Ascii models and then uses that model to analyze images on a pixel by pixel basis. The loaded models can be generated by the users or they can be loaded from a system library that we provide.

- The Image Pixels Model Selection package extends the concepts in Analyze Image Pixels to model selection. In this package the user can load a number of different models that describe the signal in a pixel and then the program will compute the posterior probability for the model. Outputs include the posterior probability for the model indicator as well as parameter maps of the parameters.

## 1.2 The Client Interface

The interface to the Bayesian Analysis software is a Java interface that runs on any machine having Java 6 or higher. Assuming the Bayesian Analysis software has been installed on a server at your site, for arguments sake lets call this machine "your.server.net," then you can bring up the interface, the client software, by issuing:

```
javaws http://your.server.net:8080/Bayes/launch.jnlp
```

where "javaws" is the Java web-start utility and comes with most Java installations, "your.server.net" should be replaced by your server name or IP address, and you should replace "8080" by the port number used by your installation, see Chapter 2 for a description of how to install the software.

If you do not have the software installed on your local machines, you can download the interface directly from Washington University:

```
javaws http://bayes.wustl.edu/Bayes/launch.jnlp
```

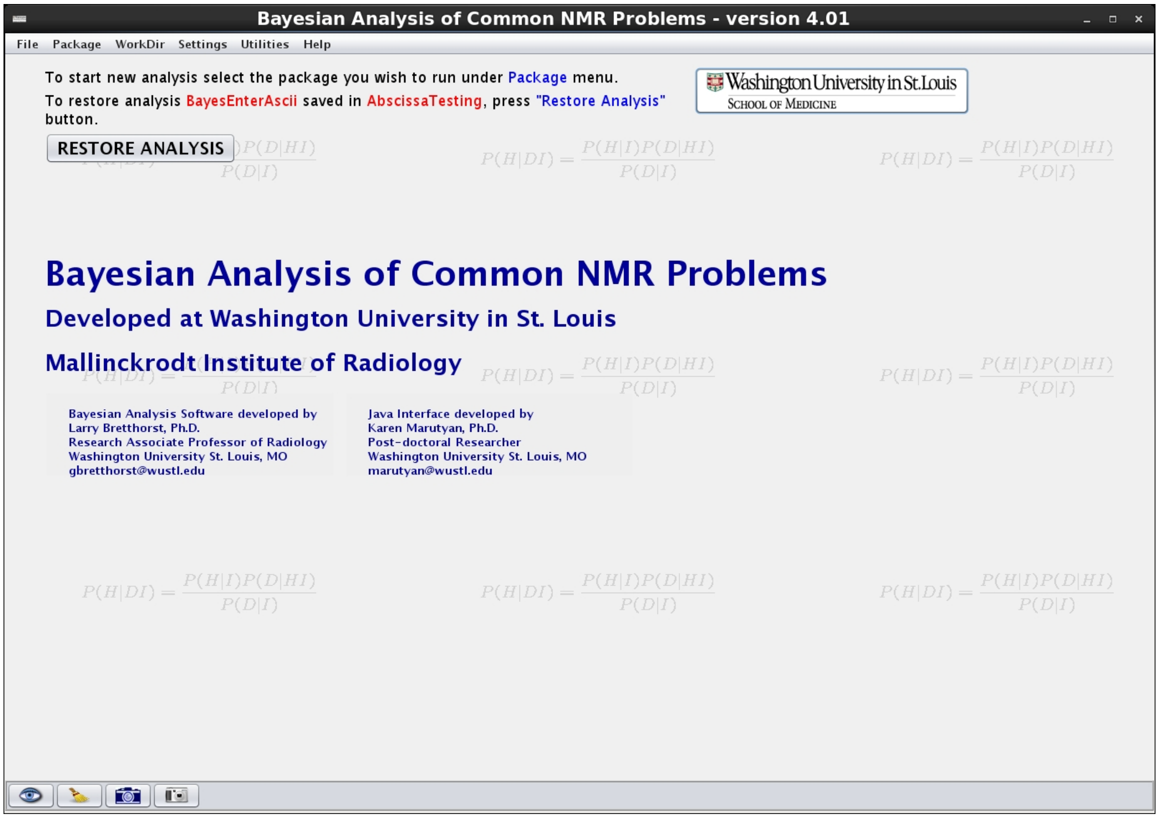
This version of the interface, will allow you to view the packages and to determine what is available. However, because the software has not been installed on one of your machines, you will not be able to run an analysis.

Assuming you use one of these to methods to start the interface, it will displays the default startup page shown in Fig. 1.1. The purpose of the startup page is to allow you to restart an analysis. When you exit the interface or changes working directories, the interface saves the current settings in a special Java properties file. When the interface start, it consults this file and determines what your last WorkDir was and how to restart that analysis. If an analysis was saved, the interface displays the messages shown in Fig. 1.1, the lines starting "To restore analysis". This line contains the name of the package that was being processed, in this case the package name was "AnalyzeImagePixels" and the analysis was saved in a WorkDir named "Given". If the **Restore Analysis** button is activated then the "Given/AnalyzeImagePixels" analysis will be restored to its previous status. When the interface finishes restoring the analysis, it will function exactly like you never exited the WorkDir or interface.

If you do not want to restore an analysis then changing the package will delete the contents of the current WorkDir and configure the WorkDir for the new package. If you do not want to change packages, but want to check on another analysis then changing the current working directory using the **WorkDir** menu will cause the interface to switch to the new WorkDir and assuming that WorkDir contains a previous analysis that analysis will be restored to its previous status.

Finally, if you wish to start a completely new analysis then selecting **WorkDir/Edit** will bring up a popup that will allow you to create a new WorkDir. After you create and join a new WorkDir the first thing you must do is to select the package you wish to use.

The global pull down menus along the top of the startup page are always present on all package interfaces, not just the startup page. They allow the user to load files, select packages, configure



To start new analysis select the package you wish to run under Package menu.
To restore analysis BayesEnterAscii saved in AbscissaTesting, press "Restore Analysis" button.

Bayesian Analysis of Common NMR Problems

Developed at Washington University in St. Louis

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Figure 1.1: The Bayesian Analysis Startup Page allows you to select what functions you wish to perform. For example you might restore an old analysis, change a setting, run one of the utility programs or select a new WorkDir or a new Bayesian Analysis package.

servers, change working directories, set options, etc. Each pull down menu has multiple functions and the following Sections explain these menus and how to go about using them.

### 1.2.1 The Global Pull Down Menus

The global pull down menus a the top of the interface are always present. They allow you to select Bayesian Analysis applications, configure servers, change WorkDir, etc. Each item across the top is a pull down menu and each menu has multiple functions. These functions are explained in detail in Section 3 Here we give a brief summary of these menus:

**Files** is pull down menu that allows you to perform various tasks involving files. For example, you can load Ascii data, FID spectral or image data and images. Additionally, you can save the current WorkDir, and you can restore a previously saved experiment. See Section 3.1.1 for more on the files submenu.

**Packages** is a pull down menu that allows you to select the Bayesian Analysis package you wish to use. Each of the packages is described in more detail in the upcoming Chapters. See Section 3.1.2 for a more extensive discussion of the packages pull down menu.

**WorkDir** is a pull down menu that allows you to select, create or delete a WorkDir. Working directories are contained within the "Bayes" directory in your home account. These directories are scratch areas used to contain the loaded data, configuration files, and the results of running an analysis. See Section 3.1.3 for a more extensive discussion of working directories.

**Settings** is a pull down menu that allows you to configure the Bayesian Analysis packages. The various menu items allow you to configure the Markov chain Monte Carlo simulations, see Section 3.1.4; add, delete and modify server settings, See Section 3.1.4; and it allows you to configure some optional features of the software.

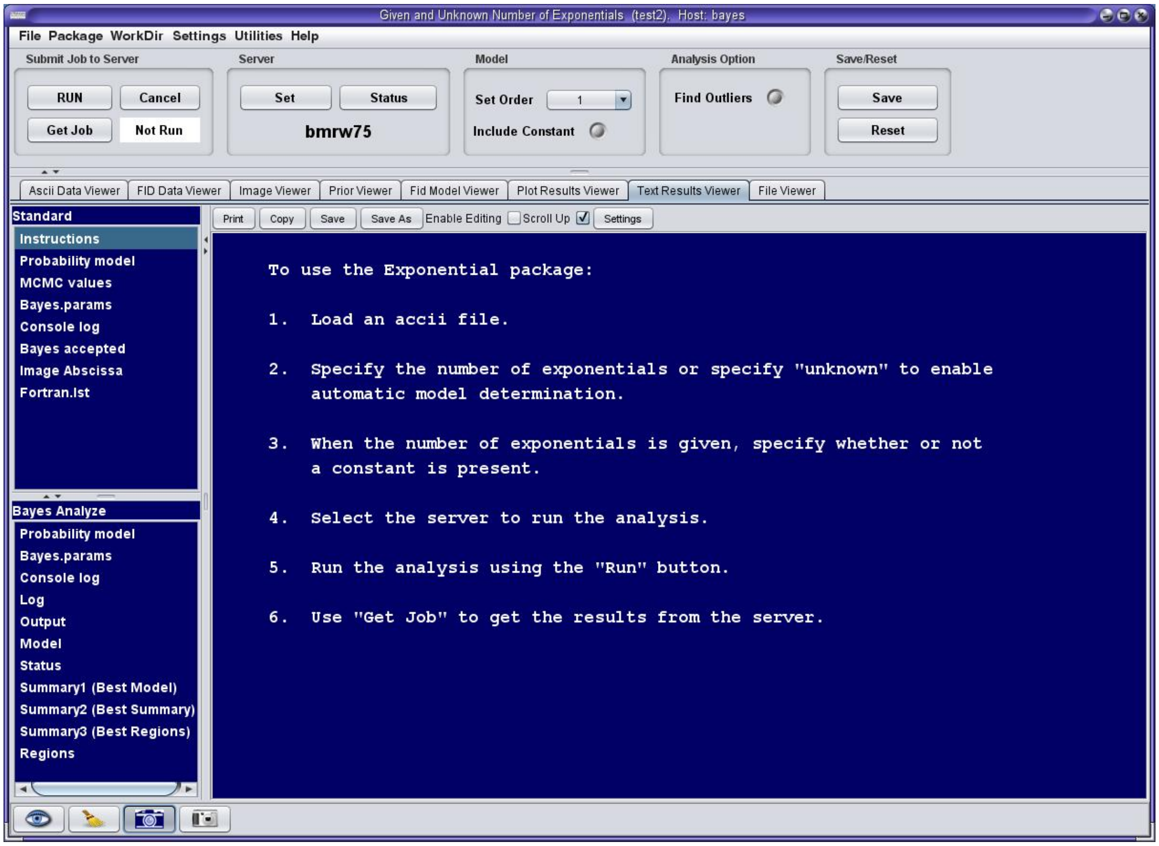
**Utilities** is a pull down menu that allows you to start a memory monitor, get information on the system you are running, and allows you to determine if there is an updated version of the Bayesian Analysis software. See Section 3.1.5 for more on the utilities.

**Help** is a pull down menu that allows you to view information about the current installation of the Bayesian Analysis software, and it allows you to visit the Bayesian Analysis Software home page.

### 1.2.2 The Package Interface

When one of the packages is selected the interface displays that package interface. For example if the Exponential package is selected, the interface shown in Fig. 1.2 is displayed. This interface is very similar to the interface of many other packages and we will use it to illustrate some of the general features of the Interface.

First, note that the global menus that were present on the Bayesian Analysis Home Page are present on all package interfaces. Second, below the global menus is an area that is used to configure a package. Each set of widgets are enclosed in a highlighted box. We are going to call these enclosed widgets, widget groups and we will name them based on the name above each group. So on the Exponential interface there are five widget groups. The first two, Submit Job to Server and Server



```
To use the Exponential package:

1.  Load an accii file.

2.  Specify the number of exponentials or specify "unknown" to enable
    automatic model determination.

3.  When the number of exponentials is given, specify whether or not
    a constant is present.

4.  Select the server to run the analysis.

5.  Run the analysis using the "Run" button.

6.  Use "Get Job" to get the results from the server.
```

Figure 1.2: When one of the Bayesian Analysis packages is selected from the “Packages” pull down menu, the appropriate interface is displayed; here the interface to the exponential package is displayed. A package interface consists of three parts: the global pull down menus along the top, the package setup widgets just below the global pull down menus, and the viewing area, the dark blue area, at the bottom.

widget groups are common to all packages. However, most packages have some variation of the five seen in the Exponential package, but some packages have more and some have less. For the exponential package here is a brief description of these widget groups:

**Submit Job to Server** is a widget group that has three buttons and one text area. This widget group is responsible for submitting jobs, checking on there status and, when necessary canceling jobs.

- The **Run** button is used to submit a job to a server. If the currently selected server is named Server1, then the Run button will submit the job to Server1 and it will change the Run Status text area to Active or Submitted depending on whether the server uses a queuing facility. When the run button is activated most of the widgets on the interface are disabled. This is to prevent the user from making changes to the configuration while a job is running.
- The **Get Job** button sends a request to the currently selected server requesting the status of the current job. If the status is other than "Run" the Run Status text area is updated with the current status and nothing else happens. If the current status is Run, the job is fetched from the server and the appropriate files are updated. Finally the Run status text area is set to Run. If for some reason the job failed, the Run Status text area is set to Error.
- The **Cancel** button will send a request to the server to cancel a job. When the server receives this request, it will determine if the job is running and if so the job is killed and the temporary work directories containing the job are removed. If the job has already finished, the temporary work directories are removed.
- The **Run Status** text area on the bottom right of the Submit Job widget group is used to display the current status of a job.

**Server** is a global widget group that has two buttons and one text area. In general terms this widget group allows you to set the current server.

- The server **Set** button allows you to set the current server. When you click on this button, a pull down menu appears containing a list of all of the servers that you have configured on the interface. Note there may be other servers, but if you have not told the interface about them, they will not appear in this pull down menu. Clicking on a server, will cause it to be set as the current server. The current server is displayed in the server name text are under this button. At the bottom of pull down menu is an item **Edit Servers** that can be used to modify your list of servers. Activating this widget will bring up a popup, Chapter 3.1.4, that allows you to modify your current servers and to add new ones if desired. This Server Edit popup is also available under the **Settings/Server Setup** menu.
- The server **Status** button will send a request for a list of jobs currently running on the server. On Linux and Sun systems this request is a simple "ps". The results of this request are displayed in the Text Viewer at the bottom of the interface.
- The current Server is displayed in the **Server Name** text area under the two button in the Server widget group.

**Model** is a widget group that is specific to the Exponential package. In the exponential package the Model widget group servers three purposes: to set the order of the exponential model to be processed, to indicate if a constant offset is present, and indicate if the number of exponentials is unknown. For a more detailed description of these widgets see the chapters on the exponential packages, Chapters 5 and 6.

**Analysis Options** is a widget group that shows up on many packages. The exact content of this widget group is specific to each package. Here there is a single widget that indicates whether or not the program is to attempt outlier detection. For more on the outlier model and how it is handled in the calculations see Chapter H.

**Reset** will resets all optional settings back to their default values.

**Save** is will bring up a popup that allows you to navigate to the location where you want to save the current WorkDir and then to Save the current WorkDir. The **Set** button will save a WorkDir.

### 1.2.3 The Viewers

After a job has been run and retrieved by the interface, the interface unpacks the result of the analysis. After unpacking the run status is set to “Run” and the various viewers located at the bottom of the interface can be used to look at the results of an analysis. These viewers are act to display various kinds of data.

The buttons along the center of the interface activate the various viewers. These Viewers are used by the interface to display different kinds of data. Because the display requirements for different types of data are very different there are many different viewers. Not all viewers show up on all packages. On the Exponential package, the viewers shown above, there are seven of these viewers, and this is pretty typical of all packages. For more information on these viewers see Chapter 3.4. Here we are just going to briefly list the viewers and note there primary function:

- The **Ascii Data Viewer** is used to display Ascii data. For more information on this viewer see Section 3.4.1.
- The **FID Data Viewer** allows you to look at both the time and frequency domain FID data. Here FID data means spectroscopic FID data. For more information on this viewer see Section 3.4.2.
- The **Image Viewer** is used to display 4dfp images. For more information on this viewer see Section 3.4.2.
- The **Prior Viewer** is used to display and set the prior probabilities used in the Bayesian calculations. For more information on this viewer see Section 3.4.4.
- The **FID Model Viewer** is used to display FID models generated by packages that process FID data. For more on this viewer see Section 3.4.5.

- The **Plot Results Viewer** is used to display the plots associated with an analysis and is the primary method for viewing the results of an analysis. For more on this viewer see Section 3.4.6.
- The **Text Results Viewer** is used to display and print the Ascii files that result from an analysis. For more on the Text Results viewer, see Section 3.4.8.
- Finally the **File Viewer** is used to view the all the files generated by analysis. For more on the Text Results viewer, see Section 3.4.9.

The overview given in this Chapter should give you some indication of what the software can do. The Java interface provides a simple user friendly way of setting up a Bayesian Analysis. After the analysis is set up the interface will automatically ship the analysis to the selected server. The Bayesian Analysis software on that server can run many different types of analysis relevant to NMR in parallel. The interface allows the user to leave an analysis while its running and then come back to that analysis at a later time and simply pick up the analysis from the point they left off. The user can determine the status of a job while its running and then fetch the job when its completed. The interface provides a convenient way of displaying the results of the analysis in graphical form and, finally, allows the user to view and print the outputs from an analysis.

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