

Bayesian Data-Analysis Toolbox  
Release 4.23, Manual Version 3

G. Larry Bretthorst  
Biomedical MR Laboratory  
Washington University School Of Medicine,  
Campus Box 8227  
Room 2313, East Bldg.,  
4525 Scott Ave.  
St. Louis MO 63110  
<http://bayes.wustl.edu>  
Email: [gbretthorst@wustl.edu](mailto:gbretthorst@wustl.edu)

September 18, 2018

## Chapter 11

# Find Resonances

There are two frequency finding programs in the Bayesian Analysis Software: Bayes Analyze, Chapter 8, and Bayes Find Resonance. Bayes Analyze is a searching algorithm that uses the residuals from the current fit, to determine if there is evidence in the data for and additional resonance. While this procedure is implemented using Bayesian probability theory, it is still an approximation to computing the full Bayesian posterior probability for the number of resonances. We implemented Bayes Analyze in this way, so that it would be very fast. However, under some conditions, Bayes Analyze will miss resonances when they are either very close together or the signal-to-noise of the resonance is very low. To solve these problems, we implemented a frequency finding program that uses Markov chain Monte Carlo to compute the posterior probability for the number of resonances. The interface to the find resonance package is shown in Fig. 11.1 To use this package, you must do the following:

**Select** the Bayes Find Resonances package from the Package menu.

**Load** the Fid data that is to be analyzed. If the Fid is arrayed, select the trace that is to be analyzed. The trace analyzed is the currently displayed trace. At the present time only a single Fid is processed by Bayes Find Resonances package.

**Select** the phase model, the choices are correlated, uncorrelated and automatic.

- If the phase model is “Common,” the all resonances have the same phase.
- If the phase model is “Independent,” the all resonances have a different phase.
- If the phase model is “Automatic,” then the Bayes Find Resonances package computes the posterior probability for the phase of each resonance.

**Check** the “Constant” box if the data contains an offset.

**Set** the first and last Fids that are to be analyzed. Note that these Fids are analyzed separately, not jointly, so you will get an analysis for each selected Fid.

**Set** the maximum number of resonances that can be included in a model.

**Select** the server that is to process the analysis.

Figure 11.1: The Find Resonances Interface With The Ethyl Ether Spectrum

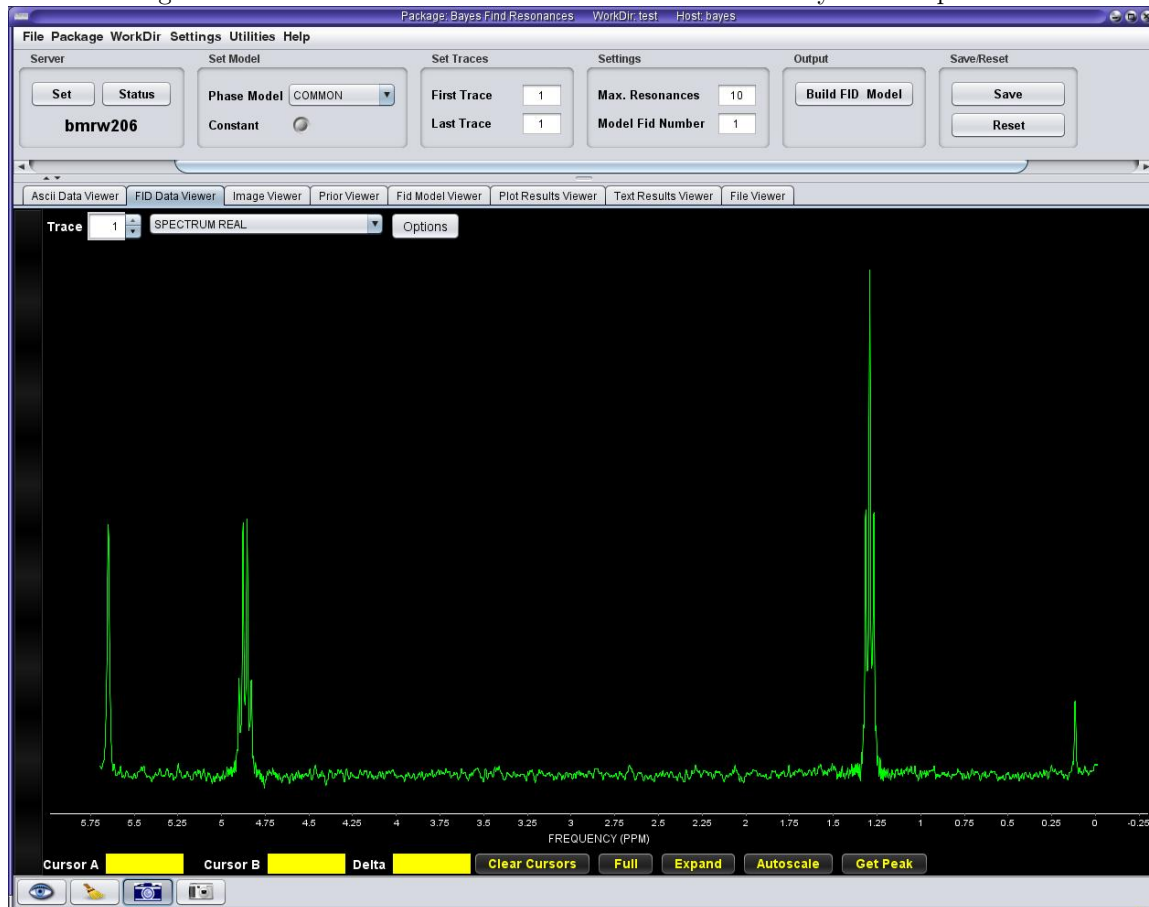


Figure 11.1: When the Find Resonances package is selected, this is the displayed interface. To use this package, load the Fid you wish to analyze. The spectrum of this Fid will be displayed in the Fid Data Viewer. Select the Fid you wish to analyze and display that Fid. At the present time only a single Fid may be processed at one time. Set the various optional feature of the model you wish to use and run the analysis. When the analysis finishes use the “Build Model” button to select and build a model of the Fid. The Fid Model Viewer can then be used to view this model.

**Check** the status of the selected server to determine if the server is busy, change to another server if the selected server is busy.

**Run** the analysis on the selected server by activating the “Run” button.

**Get** the results of the analysis by activating the “Get Job” button. If the analysis is running, this button will return the Accepted report containing the status of the current run. Otherwise, it will fetch and display the results from the current analysis.

Unlike Bayes Analyze which outputs parameter estimates computed using the values that maximized the joint posterior probability for the parameters, Bayes Find Resonances outputs mean and standard deviation parameter estimates computed from all high probability models. That is to say if the probability for the number of resonances was 50% for 9 and 50% for 10 resonances, then there will be mean and standard deviation parameter estimates for the frequencies and decay rate constants from both of these models. Additionally, Bayes Find Resonances runs multiple Fids one right after the other. Consequently, when a Fid model of the time domain data is generated, you must specify both the resonance model and the number of the Fid to model. The Fid number to model is indicated using the “Model Fid Number” entry box. If there are multiples high probability resonance models, clicking on the “Build FID Model” button will show you a list of these models and you can select which one you wish to use in generating a time domain Fid model.

## 11.1 The Bayesian Calculations

The first step in all Bayesian calculations is to define the problem. Here, the problem is essentially a parameter estimation calculations where one is estimating the frequencies, amplitudes, decay rate constants and phases of multiple exponentially decaying sinusoidal. The model will designated as  $\mathbf{M}(\mathbf{t}_i)$  where complex quantities will be in bold. Then symbolically the model which relates the complex data, model and noise is given by:

$$\mathbf{d}_i = \mathbf{M}(\mathbf{t}_i) + \mathbf{n}_i \quad (i \in \{1, \dots, N\}), \quad (11.1)$$

where  $N$  is the total number of complex data values,  $\mathbf{d}_i$  is a complex data values sampled at time  $t_i$ , and  $\mathbf{n}_i$  is a complex noise value at time  $t_i$ . The complex model  $\mathbf{M}(\mathbf{t}_i)$  is given by:

$$\mathbf{M}(\mathbf{t}_i) = [\mathbf{F}\delta(t_i) + \mathbf{C}] \delta(\nu) + \sum_{j=1}^m A_j \exp \{2\pi i f_j(t_i - t_0) - \alpha_j t_i + i\phi\delta(\xi_j) + i\phi_j[1 - \delta(\xi_j)]\} \quad (11.2)$$

where  $\mathbf{F}$  is a model of the first data value, the function  $\delta(\cdot)$  is defined below,  $\mathbf{C}$  is a complex offset,  $m$  is the unknown number of sinusoids,  $A_j$  is the amplitude of the  $j$ th sinusoid,  $f_j$  is the frequency of the  $j$ th sinusoid,  $t_0$  is a first order phase correction,  $\alpha_j$  is the decay rate constant of the  $j$ th sinusoid. The quantity “ $\phi\delta(\xi_j) + \phi_j[1 - \delta(\xi_j)]$ ” is the phase of the  $j$  sinusoid and is either a common zero order phase,  $\phi$ , or a unique phase specific to the  $j$ th sinusoid,  $\phi_j$ . Whether or not the phase is common or unique depends on the value of the indicator function  $\delta(\xi_j)$ . The indicator function  $\delta(\cdot)$  is defined as

$$\delta(\nu) = \begin{cases} 1 & \text{If } \nu = 0 \\ 0 & \text{Otherwise} \end{cases} \quad (11.3)$$

so, for example, the quantity  $\mathbf{F}\delta(t_i)$  is present only when  $t_i = 0$ . Similarly, the common phase  $\phi$  is present only when  $\xi_j = 0$ , where  $\xi_j$  is a two value binary variable defined as:

$$\xi_j = \begin{cases} 1 & \text{If the } j\text{th sinusoid has a common zero order phase} \\ 0 & \text{Otherwise} \end{cases} . \quad (11.4)$$

Here common zero phase means that several sinusoids share the same zero order phase parameter.

The value of  $\xi_j$  is under user control. If the user selects the ‘‘Common’’ phase model, then  $\xi_j = 0$  for all sinusoids and all sinusoids share the same common zero order phase parameter. If the user selects the ‘‘Independent’’ phase model, then  $\xi_j = 1$  for all sinusoids and all sinusoids have a unique zero order phase parameter  $\phi_j$ . Finally, if the user selects the phase model as ‘‘Independent’’ then the parameters  $\xi_j$  are binary variables that are simulated in the Markov chain Monte Carlo simulation, i.e., the Bayes Find Resonances package automatically determines which resonances have common zero order phase and which have a unique zero order phase.

Whether or not the constant models are present is also under user control. If the ‘‘Constant’’ check box is activated, then  $\nu$  is set equal to zero by the package and  $\delta(\nu) = 1$  and in Eq (11.2) the constant models are present. If the constant check box is not active then  $\nu = 1$  and no constants are present in Eq (11.2). However, unlike the phase model, the Bayes Find Resonances package does not simulate the binary variable  $\nu$ , this value is set by the user and the package uses the indicated value.

The Bayes Find Resonances package is a hybrid parameter estimation and model selection package. It is model selection in that it must determine how many resonances are present, and when the phase model is selected as ‘‘Independent’’ it must also estimate the binary parameters,  $\xi_j$ . So, the set of parameters estimated by Bayes Find Resonances package when all parameters are active, is:

**F** is the complex first point model, it contains two constants  $F_R$  and  $F_I$ , the real and imaginary first point parameters.

**C** is the complex constant offset model, it contains two constants  $C_R$  and  $C_I$ , which are the real and imaginary offset parameters.

$m$  is the unknown number of sinusoids in the data.

$A$  is the collection of amplitudes in the  $m$  sinusoids, so  $A \equiv \{A_1, \dots, A_m\}$ .

$f$  is the collection of frequencies in the  $m$  sinusoids, so  $f \equiv \{f_1, \dots, f_m\}$ .

$\alpha$  is the collection of decay rate constants in the  $m$  sinusoids, so  $\alpha \equiv \{\alpha_1, \dots, \alpha_m\}$ .

$t_0$  is the first order phase in in the  $m$  sinusoids.

$\xi$  is the collection of phase model indicators in the  $m$  sinusoids, so  $\xi \equiv \{\xi_1, \dots, \xi_m\}$ .

$\phi$  is the common zero order phase in the  $j$ th sinusoids when  $\delta(\xi_j) = 1$ .

$\phi_j$  is the zero order phase in the  $j$ th sinusoids when  $\delta(\xi_j) = 0$ .

We are going to designate this collection of parameters as  $\Phi$  and then proceed with the Bayesian calculations.

The Bayesian calculations are for the posterior probability for the number of resonances in the data set. This posterior probability is designated as  $P(m|DI)$ , where  $D$  represents all of the data and  $I$  stands for all of the prior information. This posterior probability is computed by application of Bayes' Theorem:

$$P(m|DI) = \frac{P(m|I)P(D|mI)}{P(D|I)} \quad (11.5)$$

where  $p(m|I)$  is the prior probability for the number of resonances,  $P(D|mI)$  is the marginal direct probability for the data given the model order and  $P(D|I)$  is a marginal direct probability for the data given only the prior information  $I$ . The direct probability for the data given only the prior information,  $P(D|I)$ , is a normalization constant and is given by:

$$\begin{aligned} P(D|I) &= \sum_{m=1}^{\text{Max}} P(Dm|I) \\ &= \sum_{m=1}^{\text{Max}} P(m|I)P(D|mI) \end{aligned} \quad (11.6)$$

where the maximum number of resonances is designated as "Max." Comparing, Eq. (11.6) to Eq. (11.5) it is easy to see that  $P(D|I)$  is a normalization constant. If we normalize the posterior probability for the number of resonances,  $P(m|DI)$ , at the end of the calculations, then Eq (11.5) becomes:

$$P(m|DI) \propto P(m|I)P(D|mI). \quad (11.7)$$

The prior probability for the number of resonances,  $P(m|I)$ , is sufficiently simplified that we could assign it a numerical value. For now we will simply leave it in this symbolic form. However, the direct probability for the data given the number of resonances and the prior information,  $P(D|mI)$ , is not yet sufficiently simplified so that its value can be assigned. To proceed with the calculation, one introduces the collection of parameters  $\Phi$  into this probability, the the direct probability for the data,  $P(D|mI)$ , the posterior probability for the number of resonances becomes

$$P(m|DI) \propto P(m|I) \int P(D\Phi|mI)d\Phi. \quad (11.8)$$

One proceeds by applying the product rule to the right-hand side of this equation:

$$P(m|DI) \propto P(m|I) \int P(\Phi|I)P(D|\Phi mI)d\Phi. \quad (11.9)$$

Factoring the prior probability for all of the parameters,  $P(\Phi|I)$  into individual prior probabilities

for each parameter, one obtains:

$$\begin{aligned}
P(m|DI) &\propto P(m|I) \int P(F_R|I)P(F_I|I)P(C_R|I)P(C_I|I) \\
&\times P(\phi|I)P(t_0|I)P(D|\Phi mI) \\
&\times \left[ \prod_{j=1}^m P(A_j|I) \right] \\
&\times \left[ \prod_{j=1}^m P(f_j|I) \right] \\
&\times \left[ \prod_{j=1}^m P(\alpha_j|I) \right] \\
&\times \left[ \prod_{j=1}^m P(\xi_j|I) \right] \\
&\times \left[ \prod_{j=1}^m P(\phi_j|I)^{\delta(\xi_j)} \right] d\Phi.
\end{aligned} \tag{11.10}$$

However, this is the marginal posterior probability for the number of resonances, and is the main output from the Bayes Find Resonances package. But the quantity sampled in the Markov chain Monte Carlo simulation is the joint posterior probability for all of the parameters. While this posterior probability is very similar, its not quite the same. The joint posterior probability for all of the parameters is given by:

$$\begin{aligned}
P(m\Phi|DI) &\propto P(m|I)P(F_R|I)P(F_I|I)P(C_R|I)P(C_I|I) \\
&\times P(\phi|I)P(t_0|I)P(D|\Phi mI) \\
&\times \left[ \prod_{j=1}^m P(A_j|I) \right] \\
&\times \left[ \prod_{j=1}^m P(f_j|I) \right] \\
&\times \left[ \prod_{j=1}^m P(\alpha_j|I) \right] \\
&\times \left[ \prod_{j=1}^m P(\xi_j|I) \right] \\
&\times \left[ \prod_{j=1}^m P(\phi_j|I)^{\delta(\xi_j)} \right]
\end{aligned} \tag{11.11}$$

which is Eq. (11.10) without the integrations. The prior probabilities are assigned as follows:

$P(m|I)$  is assigned as an Exponential prior with  $(0 \leq m \leq 50)$  where a model containing 50 resonances is a hard-coded maximum.

$P(F_R|I)$  is assigned as a bounded Gaussian prior whose range is  $\pm 6 \times$  the amplitude of the first data value and whose standard deviation is three times the magnitude of the first data value.

$P(F_I|I)$  is assigned the same as  $P(F_R|I)$  was assigned.

$P(C_R|I)$  is assigned as a bounded Gaussian whose mean is equal to the average of the last 10 real data values and whose upper and lower bounds is 5 times the mean. Finally, the standard deviation of this prior is one fifth of the prior range.

$P(C_I|I)$  is assigned like  $P(C_R|I)$  except the means and bounds are taken from the imaginary channel.

$P(\phi|I)$  is assigned a uniform prior probability ranging from zero to  $2\pi$ .

$P(t_0|I)$  essentially sets a time when the phases of all the sinusoids are the same. The prior probability for this time offset has a mean of zero, meaning that the phases are all expected to be the same at the start of the acquisition. However, we allow this parameter to range over  $\pm 5$  dwell or sampling times, i.e., the zero of time could occur the equivalent of 5 data values before the start of the acquisition and up to 5 data value past the start of acquisition. However, the standard deviation of this Gaussian prior probability is only 0.3 data values. Indicating, that while  $T_0$  is allowed to have a large range, in fact it is strongly suspected that its value is near zero.

$P(A_j|I)$  is assigned a bounded Gaussian prior probability for one of the amplitudes. Its mean is zero, its upper and lower bounds are 3 times the average magnitude of the first 10 complex data values and its standard deviation is two times that average. This prior is used for the prior probability for each resonance amplitude in the model.

$P(f_j|I)$  is assigned a uniform prior probability ranging over the entire sweep width of the data. This prior is used for the prior probability for each resonance frequency in the model.

$P(\alpha_j|I)$  is assigned a positive prior probability whose low is 0.001 in dimensionless units. The peak value is set to the current value of the “lb” parameter. The maximum value is set so that if the signal were decaying at this maximum, it will go through roughly 3 e-foldings in the first 9 data values. So the maximum value is strongly dependent on the sampling rate.

$P(\xi_j|I)$  is assigned a discrete uniform prior probability having two possible values, zero or one with zero indicating an independent phase and one indicating a common phase.

$P(\phi_j|I)$  is assigned a uniform prior probability ranging from zero to  $2\pi$ . In the above equations, [11.10](#) and [11.11](#), this probability is written as  $P(\phi_j|I)^{\delta(\xi_j)}$ , which is just a notational mechanism to indicate that the prior is either present or not. When  $\delta(\xi_j) = 1$ ,  $\xi_j = 0$ , the phase model is independent and the prior is present. Similarly, when  $\xi_j = 1$  the phase model is common and this prior is not present because the prior is raised to the zero power.

$P(D|\Phi m I)$  is the direct probability for the data given all of the parameters and the prior information and is assigned using a Gaussian prior probability for the noise. This probability is often called a likelihood or likelihood function.

The Markov chain simulation that implements this calculation targets the joint posterior probability for all of the parameters in the model, Eq. [\(11.11\)](#). It then uses Monte Carlo integration to obtain samples from the marginal posterior probability for each parameter appearing in the model. The samples from the marginal posterior probability for each parameter are then used to generate mean and standard deviation estimates of each parameter appearing in the model. Additionally, the samples are used to generate histograms. These histograms are crude estimates of the posterior probability for each parameter. In addition to outputting the histograms, the samples are also output and these samples can be used to generate Maximum Entropy histograms of the samples, see



Section (25). Finally, these samples are used to compute the posterior probability for the number of resonances, Eq. (11.10).

If there are multiple high probability models in this posterior, i.e., the posterior probability for the number of resonances,  $P(m|DI)$ , has significant weight on several values of  $m$ , then samples are drawn for each high probability model and these samples are used to generate histograms and parameter estimates given each high probability model. Consequently, then the algorithm finishes it is possible to have not one set of outputs but several. These outputs are viewed using the standard widgets. Additionally, it is possible to generate time domain Fid models for each high probability model.

## 11.2 Outputs From The Bayes Find Resonances Package

The Text outputs files from the Find Resonance packages consist of: “Bayes.prob.model,” “BayesFind-Res.mcmc.values,” “Bayes.params,” “Console.log,” “Bayes.accepted” and a “Bayes.Condensed.File.” These output files can be viewed using the Text Viewer or they can be viewed using File Viewer by navigating to the current working directory and then selecting the files. The format of the mcmc.values report is discussed in Appendix D and the other reports are discussed in Chapter ???. Additionally, the “Plot Results Viewer” can be used to view the output probability density functions. In addition to the standard data, model and residual plots there are probability density functions for the frequencies and decay rate constants, and the amplitudes for each resonance for each high probability model.

Finally, for each high probability model, there is an output “bayes.params.nnnn” and “bayes.model.nnnn” file where this file has exactly the same format as the Bayes Analyze Model file, see Chapter 8.5.7. These files are used in conjunction with the “Build FID Model” button to generate a time domain model of the input Fid data. When this button is activated the Fid and the selected bayes.model.nnnn file are sent to the server and the Bayes Model program, see Chapter 8.1 for a description of this program, is run. During this time the interface waits for the Bayes Model program to finish. When the interface detects that the model has been built, the interface fetches the model from the server, Fourier transforms the model and then displays the model using the Fid Model Viewer.

# Bibliography

- [1] Rev. Thomas Bayes (1763), “An Essay Toward Solving a Problem in the Doctrine of Chances,” *Philos. Trans. R. Soc. London*, **53**, pp. 370-418; reprinted in *Biometrika*, **45**, pp. 293-315 (1958), and *Facsimiles of Two Papers by Bayes*, with commentary by W. Edwards Deming, New York, Hafner, 1963.
- [2] G. Larry Bretthorst (1988), “Bayesian Spectrum Analysis and Parameter Estimation,” in *Lecture Notes in Statistics*, **48**, J. Berger, S. Fienberg, J. Gani, K. Krickenberg, and B. Singer (eds), Springer-Verlag, New York, New York.
- [3] G. Larry Bretthorst (1990), “An Introduction to Parameter Estimation Using Bayesian Probability Theory,” in *Maximum Entropy and Bayesian Methods*, Dartmouth College 1989, P. Fougère ed., pp. 53-79, Kluwer Academic Publishers, Dordrecht the Netherlands.
- [4] G. Larry Bretthorst (1990), “Bayesian Analysis I. Parameter Estimation Using Quadrature NMR Models” *J. Magn. Reson.*, **88**, pp. 533-551.
- [5] G. Larry Bretthorst (1990), “Bayesian Analysis II. Signal Detection And Model Selection” *J. Magn. Reson.*, **88**, pp. 552-570.
- [6] G. Larry Bretthorst (1990), “Bayesian Analysis III. Examples Relevant to NMR” *J. Magn. Reson.*, **88**, pp. 571-595.
- [7] G. Larry Bretthorst (1991), “Bayesian Analysis. IV. Noise and Computing Time Considerations,” *J. Magn. Reson.*, **93**, pp. 369-394.
- [8] G. Larry Bretthorst (1992), “Bayesian Analysis. V. Amplitude Estimation for Multiple Well-Separated Sinusoids,” *J. Magn. Reson.*, **98**, pp. 501-523.
- [9] G. Larry Bretthorst (1992), “Estimating The Ratio Of Two Amplitudes In Nuclear Magnetic Resonance Data,” in *Maximum Entropy and Bayesian Methods*, C. R. Smith et al. (eds.), pp. 67-77, Kluwer Academic Publishers, the Netherlands.
- [10] G. Larry Bretthorst (1993), “On The Difference In Means,” in *Physics & Probability Essays in honor of Edwin T. Jaynes*, W. T. Grandy and P. W. Milonni (eds.), pp. 177-194, Cambridge University Press, England.
- [11] G. Larry Bretthorst (1996), “An Introduction To Model Selection Using Bayesian Probability Theory,” in *Maximum Entropy and Bayesian Methods*, G. R. Heidbreder, ed., pp. 1-42, Kluwer Academic Publishers, Printed in the Netherlands.

- [12] G. Larry Bretthorst (1999), “The Near-Irrelevance of Sampling Frequency Distributions,” in *Maximum Entropy and Bayesian Methods*, W. von der Linden *et al.* (eds.), pp. 21-46, Kluwer Academic Publishers, the Netherlands.
- [13] G. Larry Bretthorst (2001), “Nonuniform Sampling: Bandwidth and Aliasing,” in *Maximum Entropy and Bayesian Methods in Science and Engineering*, Joshua Rychert, Gary Erickson and C. Ray Smith *eds.*, pp. 1-28, American Institute of Physics, USA.
- [14] G. Larry Bretthorst, Christopher D. Kroenke, and Jeffrey J. Neil (2004), “Characterizing Water Diffusion In Fixed Baboon Brain,” in *Bayesian Inference And Maximum Entropy Methods In Science And Engineering*, Rainer Fischer, Roland Preuss and Udo von Toussaint *eds.*, AIP conference Proceedings, **735**, pp. 3-15.
- [15] G. Larry Bretthorst, William C. Hutton, Joel R. Garbow, and Joseph J.H. Ackerman (2005), “Exponential parameter estimation (in NMR) using Bayesian probability theory,” *Concepts in Magnetic Resonance*, 27A, Issue 2, pp. 55-63.
- [16] G. Larry Bretthorst, William C. Hutton, Joel R. Garbow, and Joseph J. H. Ackerman (2005), “Exponential model selection (in NMR) using Bayesian probability theory,” *Concepts in Magnetic Resonance*, 27A, Issue 2, pp. 64-72.
- [17] G. Larry Bretthorst, William C. Hutton, Joel R. Garbow, and Joseph J.H. Ackerman (2005), “How accurately can parameters from exponential models be estimated? A Bayesian view,” *Concepts in Magnetic Resonance*, 27A, Issue 2, pp. 73-83.
- [18] G. Larry Bretthorst, W. C. Hutton, J. R. Garbow, and Joseph J. H. Ackerman (2008), “High Dynamic Range MRS Time-Domain Signal Analysis,” *Magn. Reson. in Med.*, **62**, pp. 1026-1035.
- [19] V. Chandramouli, K. Ekberg, W. C. Schumann, S. C. Kalhan, J. Wahren, and B. R. Landau (1997), “Quantifying gluconeogenesis during fasting,” *American Journal of Physiology*, **273**, pp. H1209-H1215.
- [20] R. T. Cox (1961), “The Algebra of Probable Inference,” Johns Hopkins Univ. Press, Baltimore.
- [21] André d’Avignon, G. Larry Bretthorst, Marilyn Emerson Holtzer, and Alfred Holtzer (1998), “Site-Specific Thermodynamics and Kinetics of a Coiled-Coil Transition by Spin Inversion Transfer NMR,” *Biophysical Journal*, **74**, pp. 3190-3197.
- [22] André d’Avignon, G. Larry Bretthorst, Marilyn Emerson Holtzer, and Alfred Holtzer (1999), “Thermodynamics and Kinetics of a Folded-Folded Transition at Valine-9 of a GCN4-Like Leucine Zipper,” *Biophysical Journal*, **76**, pp. 2752-2759.
- [23] David Freedman, and Persi Diaconis (1981), “On the histogram as a density estimator:  $L_2$  theory,” *Zeitschrift für Wahrscheinlichkeitstheorie und verwandte Gebiete*, **57**, 4, pp. 453-476.
- [24] W. R. Gilks, S. Richardson, and D. J. Spiegelhalter (1996), “Markov Chain Monte Carlo in Practice,” Chapman & Hall, London.

- [25] Paul M. Goggans, and Ying Chi (2004), “Using Thermodynamic Integration to Calculate the Posterior Probability in Bayesian Model Selection Problems,” in *Bayesian Inference and Maximum Entropy Methods in Science and Engineering: 23rd International Workshop*, **707**, pp. 59-66.
- [26] Marilyn Emerson Holtzer, G. Larry Bretthorst, D. André d’Avignon, Ruth Hogue Angelette, Lisa Mints, and Alfred Holtzer (2001), “Temperature Dependence of the Folding and Unfolding Kinetics of the GCN4 Leucine Lipper via  $^{13}\text{C}$  alpha-NMR,” *Biophysical Journal*, **80**, pp. 939-951.
- [27] E. T. Jaynes (1968), “Prior Probabilities,” *IEEE Transactions on Systems Science and Cybernetics*, SSC-4, pp. 227-241; reprinted in [30].
- [28] E. T. Jaynes (1978), “Where Do We Stand On Maximum Entropy?” in *The Maximum Entropy Formalism*, R. D. Levine and M. Tribus *Eds.*, pp. 15-118, Cambridge: MIT Press, Reprinted in [30].
- [29] E. T. Jaynes (1980), “Marginalization and Prior Probabilities,” in *Bayesian Analysis in Econometrics and Statistics*, A. Zellner *ed.*, North-Holland Publishing Company, Amsterdam; reprinted in [30].
- [30] E. T. Jaynes (1983), “Papers on Probability, Statistics and Statistical Physics,” a reprint collection, D. Reidel, Dordrecht the Netherlands; second edition Kluwer Academic Publishers, Dordrecht the Netherlands, 1989.
- [31] E. T. Jaynes (1957), “How Does the Brain do Plausible Reasoning?” unpublished Stanford University Microwave Laboratory Report No. 421; reprinted in *Maximum-Entropy and Bayesian Methods in Science and Engineering* **1**, pp. 1-24, G. J. Erickson and C. R. Smith *Eds.*, 1988.
- [32] E. T. Jaynes (2003), “Probability Theory—The Logic of Science,” edited by G. Larry Bretthorst, Cambridge University Press, Cambridge UK.
- [33] Sir Harold Jeffreys (1939), “Theory of Probability,” Oxford Univ. Press, London; Later editions, 1948, 1961.
- [34] John G. Jones, Michael A. Solomon, Suzanne M. Cole, A. Dean Sherry, and Craig R. Malloy (2001) “An integrated  $^2\text{H}$  and  $^{13}\text{C}$  NMR study of gluconeogenesis and TCA cycle flux in humans,” *American Journal of Physiology, Endocrinology, and Metabolism*, **281**, pp. H848-H856.
- [35] John Kotyk, N. G. Hoffman, W. C. Hutton, G. Larry Bretthorst, and J. J. H. Ackerman (1992), “Comparison of Fourier and Bayesian Analysis of NMR Signals. I. Well-Separated Resonances (The Single-Frequency Case),” *J. Magn. Reson.*, **98**, pp. 483–500.
- [36] Pierre Simon Laplace (1814), “A Philosophical Essay on Probabilities,” John Wiley & Sons, London, Chapman & Hall, Limited 1902. Translated from the 6th edition by F. W. Truscott and F. L. Emory.
- [37] N. Lartillot, and H. Philippe (2006), “Computing Bayes Factors Using Thermodynamic Integration,” *Systematic Biology*, **55** (2), pp. 195-207.

- [38] D. Le Bihan, and E. Breton (1985), “Imagerie de diffusion in-vivo par rsonance,” Comptes rendus de l’Acadmie des Sciences (Paris), **301** (15), pp. 1109-1112.
- [39] N. R. Lomb (1976), “Least-Squares Frequency Analysis of Unevenly Spaced Data,” *Astrophysical and Space Science*, **39**, pp. 447-462.
- [40] T. J. Loredo (1990), “From Laplace To SN 1987A: Bayesian Inference In Astrophysics,” in *Maximum Entropy and Bayesian Methods*, P. F. Fougere (ed), Kluwer Academic Publishers, Dordrecht, The Netherlands.
- [41] Craig R. Malloy, A. Dean Sherry, and Mark Jeffrey (1988), “Evaluation of Carbon Flux and Substrate Selection through Alternate Pathways Involving the Citric Acid Cycle of the Heart by  $^{13}\text{C}$  NMR Spectroscopy,” *Journal of Biological Chemistry*, **263** (15), pp. 6964-6971.
- [42] Craig R. Malloy, Dean Sherry, and Mark Jeffrey (1990), “Analysis of tricarboxylic acid cycle of the heart using  $^{13}\text{C}$  isotope isomers,” *American Journal of Physiology*, **259**, pp. H987-H995.
- [43] Lawrence R. Mead and Nikos Papanicolaou, “Maximum entropy in the problem of moments,” *J. Math. Phys.* **25**, 2404–2417 (1984).
- [44] K. Merboldt, Wolfgang Hanicke, and Jens Frahm (1969), “Self-diffusion NMR imaging using stimulated echoes,” *Journal of Magnetic Resonance*, **64** (3), pp. 479-486.
- [45] Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller (1953), “Equation of State Calculations by Fast Computing Machines,” *Journal of Chemical Physics*. The previous link is to the Americain Institute of Physics and if you do not have access to Science Sitations you many not be able to retrieve this paper.
- [46] Radford M. Neal (1993), “Probabilistic Inference Using Markov Chain Monte Carlo Methods,” technical report CRG-TR-93-1, Dept. of Computer Science, University of Toronto.
- [47] Jeffrey J. Neil, and G. Larry Bretthorst (1993), “On the Use of Bayesian Probability Theory for Analysis of Exponential Decay Data: An Example Taken from Intravoxel Incoherent Motion Experiments,” *Magn. Reson. in Med.*, **29**, pp. 642–647.
- [48] H. Nyquist (1924), “Certain Factors Affecting Telegraph Speed,” *Bell System Technical Journal*, **3**, pp. 324-346.
- [49] H. Nyquist (1928), “Certain Topics in Telegraph Transmission Theory,” *Transactions AIEE*, **3**, pp. 617-644.
- [50] William H. Press, Saul A. Teukolsky, William T. Vetterling and Brian P. Flannery (1992), “Numerical Recipes The Art of Scientific Computing Second Edition,” Cambridge University Press, Cambridge UK.
- [51] Emanuel Parzen (1962), “On Estimation of a Probability Density Function and Mode,” *Annals of Mathematical Statistics* **33**, 1065–1076
- [52] Karl Pearson (1895), “Contributions to the Mathematical Theory of Evolution. II. Skew Variation in Homogeneous Material,” *Phil. Trans. R. Soc. A* **186**, 343–326.

- [53] Murray Rosenblatt, "Remarks on Some Nonparametric Estimates of a Density Function," *Annals of Mathematical Statistics* **27**, 832–837 (1956).
- [54] Jeffery D. Scargle (1981), "Studies in Astronomical Time Series Analysis I. Random Process In The Time Domain," *Astrophysical Journal Supplement Series*, **45**, pp. 1-71.
- [55] Jeffery D. Scargle (1982), "Studies in Astronomical Time Series Analysis II. Statistical Aspects of Spectral Analysis of Unevenly Sampled Data," *Astrophysical Journal*, **263**, pp. 835-853.
- [56] Jeffery D. Scargle (1989), "Studies in Astronomical Time Series Analysis. III. Fourier Transforms, Autocorrelation Functions, and Cross-correlation Functions of Unevenly Spaced Data," *Astrophysical Journal*, **343**, pp. 874-887.
- [57] Arthur Schuster (1905), "The Periodogram and its Optical Analogy," *Proceedings of the Royal Society of London*, **77**, p. 136-140.
- [58] Claude E. Shannon (1948), "A Mathematical Theory of Communication," *Bell Syst. Tech. J.*, **27**, pp. 379-423.
- [59] John E. Shore, and Rodney W. Johnson (1981), "Properties of cross-entropy minimization," *IEEE Trans. on Information Theory*, **IT-27**, No. 4, pp. 472-482.
- [60] John E. Shore and Rodney W. Johnson (1980), "Axiomatic derivation of the principle of maximum entropy and the principle of minimum cross-entropy," *IEEE Trans. on Information Theory*, **IT-26** (1), pp. 26-37.
- [61] Devinderjit Sivia, and John Skilling (2006), "Data Analysis: A Bayesian Tutorial," Oxford University Press, USA.
- [62] Edward O. Stejskal and Tanner, J. E. (1965), "Spin Diffusion Measurements: Spin Echoes in the Presence of a Time-Dependent Field Gradient." *Journal of Chemical Physics*, **42** (1), pp. 288-292.
- [63] D. G. Taylor and Bushell, M. C. (1985), "The spatial mapping of translational diffusion coefficients by the NMR imaging technique," *Physics in Medicine and Biology*, **30** (4), pp. 345-349.
- [64] Myron Tribus (1969), "Rational Descriptions, Decisions and Designs," Pergamon Press, Oxford.
- [65] P. M. Woodward (1953), "Probability and Information Theory, with Applications to Radar," McGraw-Hill, N. Y. Second edition (1987); R. E. Krieger Pub. Co., Malabar, Florida.
- [66] Arnold Zellner (1971), "An Introduction to Bayesian Inference in Econometrics," John Wiley and Sons, New York.

# Index

- $A_k$  definition, 349
- $H_{j\ell}(t_i)$  definition, 349
- $\lambda_\ell$  definition, 349
- $g_{jk}$  eigenvalue, 349
- Abscissa, **437**
  - Computational, 436
  - Generating, 427
  - Loading, 39
  - Multicolumn, 437
  - Number Of Columns, 458
  - Total Data Values, 456
- Aliases, 113, **126**
- Amplitudes orthonormal definition, 349
- Analyze Image Pixel Package, **411**
  - Modification History, 413
  - Phased Images, 397
  - Reports
    - Bayes Accepted, 413
  - Using, 413
  - Viewers
    - Fortran/C Models, 411
    - Image, 411
    - Prior Probabilities, 413
  - Widgets
    - Abscissa File, 411
    - Build, 411
    - Find Outliers, 411
    - Get Statistics, 413
    - System, 411
    - User, 411
- Analyze Image Pixel Unique Package, **423**
  - Highlight
    - Abscissa, 425
    - Data, 425
  - Input Image
    - Abscissa, 423
    - Data, 423
  - Reports
    - Bayes Accepted, 425
    - Console Log, 425
    - McMC Values, 425
  - Using, 425
  - Viewers
    - Fortran/C Models, 423
    - Image, 423
    - Prior Probabilities, 425
  - Widgets
    - Build, 423
    - Find Outliers, 423
    - Get Statistics, 425
    - System, 423
    - User, 423
- Ascii Data Viewer, **53**
- Assigning Probabilities, **118**
- Bandwidth, **111, 127**
- Bayes Analyze Package, **155**
  - Levenberg-Marquardt , 171
    - Step, 194
  - Algorithm, 175
  - Amplitudes, 197, 198
  - Bayes Model, 159, 161
  - Bayesian Calculations, 167
  - Bruker, 162
  - Build BA Model, 159
  - Covariance, 174
  - Default Parameters Settings, 155
  - Error Messages, 200
  - Fid Model Viewer, 160
  - Interface, 156
  - Likelihood
    - Gaussian, 158
    - Student's  $t$ -distribution, 158

- Log File, 193, 195
- Lorentzian lineshape, 161
- Marking Resonances, 157
- Model
  - $J_o$ , 165
  - $J_p$ , 165
  - $J_s$ , 165
  - Amplitude, 163, 164
  - Bessel Function, 163
  - Constants Models, 157
  - Correlated, 157, 162, 164
  - Equation, 161, 164, 164
  - First Order Phase, 157, 162, 164
  - First Point, 162, 164
  - Gaussian, 163
  - Imaginary Constant, 164
  - Multi-Exponential, 163
  - Multiple Data Sets, 165
  - Multiplet Order, 164
  - Multiplet Orders, 164
  - Multiplets, 162
  - Multiplets of Multiplets, 164
  - Non-Lorentzian, 163
  - Offsets, 162
  - Real Constant, 164
  - Relative Amplitude, 164–166
  - Resonance Frequency, 165
  - Shim Order, 163
  - Shimming, 166
  - Shimming Order, 164
  - Uncorrelated, 157, 162, 164
  - Zero Order Phase, 157, 162, 164
- Model Interface, 160
- Multiplets, 158
- Newton-Raphson, 171
- Noise File, 158
- Noise Standard Deviation, 158
- Outputs
  - Bayes.accepted File, 177
  - bayes.log.nnnn File, 177, 193, 193
  - bayes.model.nnnn File, 177, 185, 197, 197
  - bayes.noise File, 180
  - bayes.noise.nnnn File, 158, 180
  - bayes.output.nnnn File, 176, 186, 186
  - bayes.params File, 176, 177
  - bayes.params.nnnn File, 176, 177, 177
  - bayes.probabilities.nnnn File, 177, 190, 190
  - bayes.status.nnnn File, 177, 196, 200
  - bayes.summary1.nnnn File, 177, 198, 198
  - bayes.summary2.nnnn File, 177, 199, 199
  - bayes.summary3.nnnn File, 177, 200, 200
  - Global Parameters, 182, 183
  - Model File, 184
  - Probabilities file, 191
  - Zero Order Phase, 182
- Parameter File
  - Activate Shims, 180
  - Analysis Directory, 178
  - By Fid, 181
  - Data Type, 180
  - Default Model, 181
  - Directory Organization, 180
  - Fid Model Name, 178
  - File Version, 178
  - First Fid, 181
  - First Order Phase, 180, 183
  - Imaginary Constant, 184
  - Last Fid, 181
  - lb, 182
  - Maximum Candidates, 182
  - Maximum New Resonances, 182
  - Model Fid Number, 181
  - Model Name, 184
  - Model Names, 181
  - Model Number, 184
  - Model Points, 181
  - Multiplets of Multiplets, 185
  - Noise Start, 181
  - Numerical Parameters, 178
  - Output Format, 180
  - Prior Odds, 182
  - Procpair, 178
  - Real Constant, 184
  - Relative Amplitude, 183
  - Resonance Model, 185
  - Shim Order, 182
  - Spectrometer Frequency, 182
  - Text Parameters, 178
  - Total Complex Data Values, 181
  - Total Data Values, 181
  - Total Sampling Time, 182
  - True Reference, 182



- Units, 180
- Use Noise StdDev, 180
- User Reference, 182
- Prior Probabilities, 167
- Probabilities File, 191
- Product Rule, 168
- Relative Amplitude, 167
- Remove Resonances, 159
- Reports
  - Bayes Status, 155
- Save/Reset, 159
- Search, 166
  - Levenberg-Marquardt , 166
- Short Parameter Description, 195
- Siemens, 162
- Status File, 196
- Steepest Descents, 173
- Sum Rule, 168
- Summary File, 198
- Summary Reports, 176
- Summary2, 199
- Summary3, 201
- Units, 161
- Using, 157
- Varian/Agilent, 162
- Widgets, 155
  - By, 158, 176
  - First Point, 157, 163
  - From, 158, 176
  - Imag Offset, 163
  - Imaginary Offset, 157
  - Mark, 159
  - Max New Res, 157
  - New, 159
  - Noise, 158
  - Phase, 157
  - Primary, 158
  - Real Offset, 157, 163
  - Remove, 159
  - Remove All, 159
  - Reset, 159, 193
  - Restore, 159
  - Save, 159
  - Secondary, 159
  - Shim Order, 157, 163
  - Signal, 158
  - To, 158, 176
- Bayes Find Resonances Package, **239**
  - Bayesian Calculations, 241
  - Current Fid, 239
  - Model Equation, 241
  - Number of data sets, 239
  - Phase Model
    - Automatic, 239, 242
    - Common, 239, 242
    - Independent, 239, 242
  - Prior Probabilities, 243–245
  - Reports
    - Bayes Accepted, 241, 246
    - Condensed, 246
    - Console log, 246
    - MCMC Values, 246
    - Prob Model, 246
  - Using, 239, 241
  - Viewers
    - Fid Data, 240
    - Fid Model, 240, 246
    - File, 246
    - Plot Results, 246
    - Text, 246
  - Widgets
    - Build FID Model, **240, 241, 246**
    - Constant, 239, 242
    - First Trace, 239
    - Last Trace, 239
    - Model Fid Number, 241
    - Phase Model, 239, 242
- Bayes Home Directory, 45, **49**
- Bayes Manual pdf, 469
- Bayes Metabolite Package
  - Widgets
    - Shift Left, 222
    - Shift Right, 222
- Bayes Metabolite Package, **219**
  - Aligning Resonances, 221
  - Bayesian Calculation, 225
  - Metabolite Locations, 221
  - Model Equation, 223
  - Reports
    - Bayes Accepted, 221, 238
    - Condensed, 238
    - Console log, 238

- McMC Values, [238](#)
- Prob Model, [238](#)
- Viewers
  - Fid Data, [219](#)
  - Fid Model, [221](#), [236](#)
  - File, [222](#), [238](#)
  - Metabolite, [221](#)
  - Plot Results, [238](#)
  - Text, [238](#)
- Widgets
  - Fid Model, [221](#)
  - Fid Model Viewer, [221](#)
  - Load System Metabolite File, [219](#)
  - Load System Resonance File, [221](#)
  - Load User Metabolite File, [219](#)
  - Load User Resonance File, [221](#)
  - Shift Left, [221](#)
  - Shift Right, [221](#)
- Bayes Model, [159](#), [159](#)
- Bayes Test Data Package, [427](#)
  - Parameters, [431](#)
  - Reports
    - Bayes Accepted, [428](#)
    - Condensed, [429](#)
    - McMC Values, [429](#), [431–433](#)
  - Viewers
    - Fortran/C Models, [427](#)
    - Image, [428](#)
    - Prior Probabilities, [427](#)
    - Text Data, [430](#)
    - Text Results, [429](#)
  - Widgets
    - # Images, [427](#)
    - # Slices, [427](#)
    - Abscissa, [427](#)
    - ArrayDim, [427](#)
    - Build, [427](#)
    - Get Job, [428](#)
    - Max Value, [427](#)
    - Noise SD, [427](#)
    - Parameter Ranges, [428](#)
    - Pe, [427](#)
    - Ro, [427](#)
    - Run, [428](#)
    - Set (server), [428](#)
    - Status, [428](#)
- Bayes' Theorem, [100](#), [139](#), [145](#), [153](#), [167](#), [211](#), [226](#), [243](#), [252](#), [261](#), [269](#), [278](#), [288](#), [295](#), [306](#), [314](#), [315](#), [317](#), [318](#), [331](#), [333](#), [343](#), [370](#), [399](#), [407](#), [439](#)
- Bayes.accepted
  - Body, [77](#)
  - Header, [76](#)
- Behrens-Fisher Package, [311](#)
  - Bayesian Calculations
    - Derived Probabilities, [320](#)
    - Different Mean And Same Variance, [318](#)
    - Different Mean And Variance, [319](#)
    - Parameter Estimation, [321](#)
    - Same Mean And Different Variance, [317](#)
    - Same Mean And Variance, [315](#)
  - Model Equation
    - Different Mean And Same Variance, [318](#)
    - Different Mean And Variance, [319](#)
    - Same Mean And Different Variance, [317](#)
    - Same Mean And Variance, [315](#)
  - Number of data sets, [311](#)
  - Parameter Listing, [323](#)
  - Prior Probabilities
    - Different Mean And Same Variance, [318](#)
    - Different Mean And Variance, [319](#)
    - Same Mean And Different Variance, [317](#)
    - Same Means And Same Variance, [315](#)
  - Reports
    - Bayes Accepted, [311](#), [322](#)
    - Condensed, [322](#)
    - Console Log, [322](#), [323](#)
    - McMC Values, [322](#), [323](#)
    - Prob Model, [322](#)
  - Using, [311](#)
  - Viewers
    - File, [322](#)
    - Plot Results, [322](#), [324](#)
    - Prior Probabilities, [311](#)
    - Text, [322](#)
  - Widgets
    - None, [311](#)
- Big Endian, [471](#), [473](#)
- Big Magnetization Transfer Package, [259](#)
  - Bayesian Calculations, [259](#)
  - Files
    - Bayes Analyze, [264](#)

- Fid, [263](#)
- Peak Pick, [262](#)
- Model Equation, [261](#)
- Number of data sets, [259](#)
- Prior Probabilities, [261](#)
- Reports
  - Bayes Accepted, [259](#), [262](#)
  - Condensed, [262](#)
  - Console log, [262](#)
  - McMC Values, [262](#)
  - Prob Model, [262](#)
- Using, [259](#)
- Viewers
  - Ascii Data, [259](#)
  - File, [262](#)
  - Prior Probabilities, [259](#)
  - Text, [262](#)
- Widgets
  - Find Outliers, [259](#)
- Big Peak/Little Peak Package, [207](#)
- Bayesian Calculations, [209](#)
- Fid Analyzed, [207](#)
- Model Equation, [210](#)
  - Metabolites, [209](#)
  - Solvent, [210](#)
- Number of data sets, [207](#)
- Prior Probabilities
  - Metabolite, [207](#)
  - Solvent, [207](#)
- Removing Resonances, [207](#)
- Reports
  - Bayes Accepted, [209](#), [216](#)
  - Condensed, [216](#)
  - Console log, [216](#)
  - McMC Values, [216](#)
  - Prob Model, [216](#)
- Using, [207](#)
- Viewers
  - File, [216](#)
  - Model, [209](#)
  - Plot Results, [216](#)
  - Prior Probabilities, [207](#)
  - Text, [216](#)
- Widgets
  - Metabolite, [207](#)
  - Solvent, [207](#)
- Binned Density Function Estimation, [355](#)
- Binned Histogram Package
  - Reports
    - Bayes Accepted, [357](#)
  - Viewers
    - Ascii, [355](#)
- Binned Histograms Package
  - Using, [357](#)
  - Viewers
    - Prior Probabilities, [355](#)
- Bloch-McConnell Equations, [267](#), [277](#)
- Changing the Bayes Home Directory, [469](#)
- Compilers, [29](#)
  - CC, [29](#), [455](#)
  - Fortran, [29](#), [455](#)
- Correlations, [91](#)
- Diffusion Tensor Package, [247](#)
  - Ascii File Formats, [247](#), [254](#), [255](#)
  - Bayesian Calculations, [249](#)
  - Prior Probabilities
    - $\Delta$ , [254](#)
    - $\Gamma$ , [254](#)
    - $\delta$ , [254](#)
    - $\sigma$ , [253](#)
  - Amplitudes, [253](#)
  - Eigenvalues, [253](#)
  - Euler Angles, [253](#)
  - Likelihood, [253](#)
  - Parameter, [254](#)
- Reports
  - Bayes Accepted, [247](#), [255](#)
  - Condensed, [255](#)
  - Console log, [255](#)
  - McMC Values, [255](#)
  - Prob Model, [255](#)
- Symmetries, [253](#)
- Using, [247](#)
- Viewers
  - File, [247](#), [255](#)
  - Plot Results, [255](#)
  - Prior Probabilities, [247](#), [253](#)
  - Text, [255](#)
- Widgets
  - Abscissa Options, [248](#)

- Find Outliers, [247](#)
- Include Constant, [247](#), [248](#), [255](#)
- Tensor Number, [247](#), [248](#), [255](#)
- Use b Matrix, [255](#)
- Use b Vectors, [255](#)
- Use g Vectors, [254](#)
- Discrete Fourier Transform, [110](#), [113](#), [123](#)
- Enter Ascii Model Package, [329](#)
  - Bayesian Calculations, [332](#)
    - Marginalization, [332](#)
    - No Marginalization, [331](#)
  - Fortran/C Models, [330](#), [335](#)
  - Model Equation
    - Marginalization, [331](#)
    - No Marginalization, [331](#)
  - Output Names
    - Derived, [335](#)
    - Parameters, [335](#)
  - Reports
    - Bayes Accepted, [331](#), [335](#)
    - Bayes Params, [335](#)
    - Condensed, [335](#)
    - Console log, [335](#)
    - McMC Values, [335](#)
    - Prob Model, [335](#)
  - Using, [331](#)
  - Viewers
    - Ascii Data, [329](#)
    - File, [335](#)
    - Fortran/C Models, [329](#)
    - Plot Results, [335](#)
    - Prior Probabilities, [329](#)
    - Text, [335](#)
  - Widgets
    - Build, [329](#)
    - Find Outliers, [329](#)
    - System, [329](#)
    - User, [329](#)
- Enter Ascii Model Selection Package, [341](#)
  - Bayesian Calculations
    - Marginalization, [346](#)
    - No Marginalization, [344](#)
  - Fortran/C Models, [341](#), [343](#), [353](#)
  - Model Equation, [343](#)
    - No Marginalization, [343](#)
    - With Marginalization, [347](#)
  - Output Names
    - Derived, [354](#)
    - Parameters, [353](#)
  - Reports
    - Bayes Accepted, [343](#), [353](#)
    - Condensed, [353](#)
    - Console log, [353](#)
    - McMC Values, [353](#)
    - Params File, [353](#)
    - Prob Model, [353](#)
  - Using, [343](#)
  - Viewers
    - Ascii Data, [341](#)
    - File, [353](#)
    - Fortran/C Models, [341](#)
    - Plot Results, [353](#)
    - Prior Probabilities Not Used, [341](#)
    - Text, [353](#)
  - Widgets
    - Build Not Used, [341](#)
    - Find Outliers, [341](#)
    - System, [341](#)
    - User, [341](#)
- Errors In Variables Package, [303](#)
  - Ascii File Formats
    - Errors In X and Y Known, [303](#), [309](#)
    - Errors In X Known, [303](#), [309](#)
    - Errors In Y Known, [303](#), [309](#)
    - Errors Unknown, [303](#), [309](#)
  - Bayesian Calculations, [305](#)
  - Data Error Bars, [303](#)
  - Files
    - Ascii, [303](#)
    - Bayes Analyze, [303](#)
    - Peak Pick, [303](#)
  - Model Equation, [305](#)
  - Number of data sets, [303](#)
  - Reports
    - Bayes Accepted, [305](#), [309](#)
    - Condensed, [309](#)
    - Console log, [309](#)
    - McMC Values, [309](#)
    - Prob Model, [309](#)
  - Using, [305](#)
  - Viewers

- Ascii Data, **303**
  - File, **309**
  - Plot Results, **309**
  - Text, **309**
- Widgets
  - Given Errors In, **303**
  - Order, **303**
- Exponentials
  - Given Package, **137**
  - Inversion Recovery Package, **151**
  - Magnetization Transfer Package, **267**
  - Unknown Number of Package, **143**
- Fid Data Viewer, **53**
- Fid Model Viewer, **68**
- File Format
  - Ascii, **436**
- File Viewer, **80**
- Files
  - 4dfp, **59, 428, 430, 470, 471**
    - Header, **473**
    - Reading, **471**
  - Abscissa, **39, 77, 470**
  - afh, **53**
  - ASCII, **35, 36**
  - Ascii, **53, 54, 435**
    - k*-space, **437**
    - Abscissa, **435, 436, 437**
    - Data, **435**
    - Image, **436**
  - Bayes Analyze, **36**
  - Bayes.accepted, **51, 76**
  - Bayes.params, **76, 79**
  - Bayes.prob.model, **447**
  - BayesManual.pdf, **469**
  - Condensed, **77, 78**
  - Console.log, **76, 79, 465**
  - dir.info, **470**
  - fid, **470, 470**
    - ASCII, **36**
    - ffh, **56**
    - Model, **68, 70**
    - procpa, **470**
    - Siemens Raw, **36**
    - Siemens Rda, **36**
    - Spectroscopic, **53**
    - Varian fid, **36**
  - Fortran/C Models, **42, 455, 457, 458, 465–467**
  - Images
    - 4dfp, **38**
    - Binary, **38**
    - Bruker 2dseq, **38**
    - Bruker stack, **38**
    - DICOM, **38**
    - FDF, **38**
    - Multi-Column Text, **38**
    - Siemens IMA, **38**
  - k*-space
    - Text, **36**
    - Varian fid, **36**
  - mcmc.values, **76, 449**
  - Model Listing, **77**
  - prob.model, **76**
  - procpa, **470**
  - Raw, **36**
  - RDA, **36**
  - Statistics, **65**
  - System.err.txt, **469**
  - System.out.txt, **469**
  - Varian fid, **36**
  - WaterViscosityTable, **469**
- Fortran/C Model Viewer, **93**
  - Popup Editor, **93**
- Fortran/C Models, **42, 330, 335, 353, 455**
  - Abscissa, **463**
  - Body, **463**
    - Abscissa, **457**
  - Declarations, **462**
  - Derived Parameters, **457, 459, 463**
  - Edit/Create New Model, **42, 455**
  - I/O, **464**
  - Marginalization, **464**
    - $G_j(\Omega, t_i)$ , **464**
    - Amplitude Range, **465**
    - Example, **465, 466**
    - Model Vectors, **465**
    - Ordering Amplitudes, **465**
    - Parameter File, **465, 467**
    - Parameter Order, **465**
    - Parameters, **465**
- Model Files, **455**

- Model Selection, 464
- No Marginalization, 457
  - $S(t_i)$ , 455
  - Example, 456
- Parameter File, 458, 459, 465
- Parameters, 463
- Signal, 463
- Subroutine Interface, 460
  - Abscissa, 462
  - Current Set, 460
  - Derived Parameters, 461
  - Maximum No Of Data Values, 461
  - Number Of Abscissa Columns, 461
  - Number Of Data Columns, 461
  - Number Of Derived Parameters, 461
  - Number Of Model Vectors, 461
  - Number Of Parameters, 460
  - Parameters, 461
  - Signal, 462
  - Total Complex Data Values, 461
- Subroutines and Functions, 464
- Frequency Estimation, 114, 132
- Given Exponential Package, 137
  - Bayesian Calculations, 140
  - Files
    - Ascii, 137
    - Bayes Analyze, 137
    - Peak Pick, 137
  - Model Equation, 139
  - Number of data sets, 139
  - Prior Probabilities, 139–141
  - Reports
    - Bayes Accepted, 137, 141
    - Condensed, 141
    - Console log, 141
    - McMC Values, 141
    - Prob Model, 141
  - Symmetries, 141, 148
  - Using, 137
  - Viewers
    - File, 141
    - Plot Results, 141
    - Prior Probabilities, 137, 139
    - Text, 141
  - Widgets
- Constant, 137, 139
- Find Outliers, 137
- Given Order, 27
- Include Constant, 27
- Order, 137, 139
- Given Polynomial Order Package, 285
  - Bayesian Calculations, 288
  - Files
    - Ascii, 285
    - Bayes Analyze, 285
    - Peak Pick, 285
  - Gram-Schmidt, 287
  - Model Equation, 287
  - Number of data sets, 285
  - Prior Probabilities, 289
  - Reports
    - Bayes Accepted, 285, 291
    - Condensed, 291
    - Console log, 291
    - McMC Values, 291
    - Prob Model, 291
  - Scatter Plots, 292
  - Using, 285
  - Viewers
    - File, 290
    - Plot Results, 291
    - Text, 290
  - Widgets
    - Set Order, 285
- Histograms
  - Binned, 381
  - Kernel Density, 381
- Image Model Selection Package, 415
  - Abscissa, 415
  - Fortran/C Models, 415, 417
  - Reports
    - Bayes Accepted, 417
  - Using, 417
  - Viewers
    - Fortran/C Models, 415
    - Image, 415
  - Widgets
    - Noise SD, 415
    - System, 415

- Use Gaussian, 415
- User, 415
- Image Viewer, 59
- Images
  - Flip
    - Horizontal, 63
    - Vertical, 63
  - Grayscale, 63
  - ImageJ, 63
  - Original, 63
- Inversion Recovery Package, 151
  - Bayesian Calculations, 153
  - Model Equation, 153
  - Number of data sets, 153
  - Prior Probabilities, 153
  - Reports
    - Bayes Accepted, 151, 154
    - Condensed, 154
    - Console Log, 154
    - McMC Values, 154
    - Prob Model, 154
  - Using, 151
  - Viewers
    - Plot Results, 154
    - Prior Probability, 151
  - Widgets
    - Find Outliers, 151
- Kernel Density Function Package, 361
  - Ascii File Format, 361
  - Bayesian Calculations, 369
  - Data Requirements, 361
  - Data, Model And Residuals, 369
  - Kernels, 369
    - Biweight, 362
    - Cosine, 362
    - Epanechnikov, 362
    - Exponential, 362
    - Gaussian, 362, 370
    - nonnegative, 361
    - Real Valued, 361
    - Triangular, 362
    - Tricube, 362
    - Triweight, 362
    - Uniform, 362
  - Likelihood, 371
  - Number of data sets, 364
  - Plots
    - Expected Density Function, 367, 368
    - Mean Density Function, 367, 368
    - Posterior Probability for the Kernel Type, 365
    - Posterior Probability for the Number Of Kernels, 366
    - Scatter Plots of Model Averaged Density Function, 368
    - Standard Deviation of the Mean Density Function, 367, 368
  - Prior Probabilities
    - Kernel Center, 371
    - Kernel Smoothing Parameter, 371
    - Kernel Type, 370
    - Number Of Kernels, 370
  - Reports
    - Bayes Accepted, 364
    - Condensed, 372
    - McMC Values, 372
    - Prob Model, 372
  - Using, 364
  - Viewers
    - Ascii, 361
  - Widgets
    - Kernel Type, 364
    - Output Size, 364
- Levenberg-Marquardt, 171
- Linear Phasing Package, 395, 409
  - Interface, 397
  - Model Equation, 398
  - Widgets
    - cf, 403
    - Display, 403
    - Display Array Element, 403
    - fn, 403
    - fn1, 403
    - Image Type, 402
    - Load An Image, 402
    - np, 403
    - nv, 403
    - Process, 403
  - Load Working Directory, 33
  - Logical Independence, 117

- Magnetization Transfer Kinetics Package, **275**
  - Arrhenius Plot, **281**
  - Bayesian Calculation, **278**
  - Boltzmann's Constant, **277**
  - Eyring Equation, **275, 276, 277, 280**
  - Model Equation, **277**
  - Plank's Constant, **277**
  - Prior Probabilities, **279**
  - Reports
    - Bayes Accepted, **277, 281**
    - Condensed, **281**
    - Console log, **281**
    - McMC Values, **281**
    - Prob Model, **281**
  - Sum and Difference Variables, **280**
  - Transmission coefficient, **277**
  - Universal Gas Constant, **277**
  - Using, **277**
  - van't Hoff Plot, **281**
  - Viewers
    - Ascii File, **275**
    - File, **281**
    - Prior Probabilities, **275**
    - Text, **281**
  - Widgets
    - Load, **275, 281**
    - Set, **275**
    - Uncertainty, **275**
- Magnetization Transfer Package, **265**
  - Bayesian Calculations, **267**
  - Files
    - Ascii, **265**
    - Bayes Analyze, **265**
    - Inversion Recovery, **272**
    - Peak Pick, **265**
  - Model Equation, **267**
  - Number of data sets, **265**
  - Prior Probabilities, **265, 270**
  - Reports
    - Bayes Accepted, **267, 272**
    - Condensed, **272**
    - Console log, **272**
    - McMC Values, **272**
    - Prob Model, **272**
  - Three Column Data, **265**
  - Using, **267**
- Viewers
  - Ascii Data, **265**
  - Fid Data, **272**
  - File, **271**
  - Plot Results, **262, 272, 281**
  - Prior Probabilities, **265**
  - Text, **271**
- Widgets
  - Find Outliers, **265**
- Marginalization, **100**
  - Bayes Analyze Package, **174**
  - Behrens-Fisher, **315**
  - Big Magnetization Transfer, **261**
  - Big Peak/Little Peak, **211**
  - Diffusion Tensors, **252**
  - Enter Ascii Model Package, **331**
  - Errors In Variables, **306**
  - Fortran/C Models, **464**
  - Given Exponential, **139**
  - Inversion Recovery, **153**
  - Linear Phasing, **399**
  - Magnetization Transfer, **269**
  - Magnetization Transfer Kinetics, **278**
  - Metabolic Analysis, **225**
  - Nonexhaustive Hypotheses, **101**
  - Nuisance Hypotheses, **100**
  - Nuisance Parameter, **100**
  - Unknown Number of Exponentials, **146**
- Markov chain Monte Carlo, **132, 439**
  - Acceptance Rate, **444**
  - Annealing Schedule, **91, 442**
    - Dynamic, **443**
    - Linear, **442**
  - Killing Simulations, **443**
  - Maximum Posterior Probability, **91**
  - Metropolis-Hastings, **439**
  - Mixing, **91**
  - Monte Carlo Integration, **440**
  - Multiple Simulations, **441**
  - Posterior Probability, **440**
  - Random Number Generators, **440**
  - Repeats, **91**
  - Sampling, **91**
  - Simulated Annealing, **442**
  - the Proposal, **444**



- MaxEnt Density Function Estimation Package, **373**
  - Data Requirements, **381**
  - Plots
    - Contour/Scatter, **375, 379**
    - Number Of Multipliers, **375, 378**
  - Reports
    - Bayes Accepted, **375**
    - Console Log, **375**
  - Using, **375**
  - Viewers
    - Ascii, **373**
    - Plot, **375, 378**
    - Prior Probabilities, **373**
  - Widgets
    - Histogram Size, **373**
    - Order, **373**
- Maximum Entropy Method Of Moments, **102, 377, 381**
  - Advantages, **386**
  - Problems, **386**
  - Review, **381**
- Maximum Entropy Method Of Moments Package
  - Bayesian Calculations, **387**
  - Plots
    - Data, Model and Residuals, **380**
- Menus
  - Files, **24, 35**
    - 4dfp, **37, 38**
    - Abscissa, **35, 39**
    - ASCII, **35, 36**
    - Binary, **38**
    - Bruker, **37**
    - Bruker 2dseq, **38**
    - Bruker Stack, **38**
    - DICOM, **37, 38**
    - FDF, **37, 38**
    - fid, **36, 37**
    - General Binary, **37**
    - Images, **35**
    - Import Working Directories in Batch, **40**
    - Import Working Directory, **40**
    - Load Images, **36, 37, 59**
    - Load Working Directory, **35**
    - Multi-Column Text, **37, 38**
    - Save Working Directory, **35, 39**
  - Siemens IMA, **37, 38**
  - Single-Column Text, **38**
  - Spectroscopic Fid, **35**
  - Test Data, **35, 39**
  - Text k-space, **36**
  - Text k-space fid, **37**
  - User Manual, **35, 39**
- Help, **24**
- Packages, **22, 24, 33, 40**
- Settings, **46**
  - Add Server, **48**
  - Auto Configure Server, **48**
  - MCMC Parameters, **24, 46, 48**
  - Min Annealing Steps, **48, 48**
  - Port number, **48**
  - Preferences, **49, 63**
  - Remove Server, **48, 49**
  - Repetitions, **46, 48**
  - Server Name, **48**
  - Server Setup, **24, 26, 48**
  - Set Window Size, **49**
  - Simulations, **46, 48**
  - View Server Installation Info, **48, 49**
- Spectroscopy fid, **36**
- Utilities, **24, 50**
  - Memory Monitor, **50**
  - Software Updates, **50**
  - System Information, **50**
- WorkDir
  - Creating, **22, 33, 46**
  - Deleting, **22, 33, 46**
  - List, **24, 46**
  - Loading, **46**
  - Name, **46**
  - Popup, **47**
- Model Comparison
  - Big Peak/Little Peak Package, **211**
- model orthonormal definition, **349**
- Mouse
  - Control-left, **59**
- Fid Data Viewer
  - Left, **56**
  - Right, **56**
  - Shift-left, **59**
- Multiplets
  - J-Coupling

- Center, [159](#)
- Primary, [159](#)
- Secondary, [159](#)
- Newton-Raphson, [171](#)
- Noise Standard Deviation, [64](#)
- Non-Linear Phasing Package, [405](#)
  - Calculations, [407](#)
  - Model Equation, [405](#), [407](#)
  - Widgets
    - Process, [409](#)
    - Write Ascii images, [409](#)
    - Write imaginary images, [409](#)
- Nuisance Parameter, [100](#), [115](#), [135](#)
- Nyquist Critical Frequency, [111](#), [127](#)
- orthonormal, [349](#)
- Outliers, [475](#)
  - Mean Parameter, [477](#)
  - Model, [475](#)
  - Prob Number of, [476](#)
  - Proposal, [475](#)
  - Red dot, [477](#)
  - Weighted Average, [477](#)
- Packages
  - Analyze Image Pixel Unique, [423](#)
  - Bayes Analyze, [20](#), [43](#), [57](#), [155](#), [200](#)
  - Bayes Find Resonances, [21](#), [239](#)
  - Bayes Test Data, [427](#)
  - Behrens-Fisher, [21](#), [44](#), [311](#)
  - Big Magnetization Transfer, [20](#), [43](#), [259](#)
  - Big Peak/Little Peak, [20](#), [43](#), [207](#)
  - Binned Density Function Estimation, [355](#)
  - Binned Histograms, [21](#), [44](#)
  - Diffusion Tensors, [20](#), [40](#), [247](#)
  - Enter ASCII Model, [42](#)
  - Enter Ascii Model, [20](#), [329](#)
  - Enter ASCII Model Selection, [42](#)
  - Enter Ascii Model Selection, [20](#), [341](#)
  - Errors In Variables, [21](#), [44](#), [303](#)
  - Find Resonances, [43](#)
  - Given Exponential, [20](#), [40](#), [137](#)
  - Given Polynomial Order, [285](#)
  - Image Model Selection, [415](#)
  - Image Pixel, [21](#), [45](#), [411](#)
  - Image Pixel Model Selection, [22](#), [45](#)
  - Inversion Recovery, [20](#), [40](#), [151](#)
  - Kernel Density Function, [361](#)
  - Linear Phasing, [21](#), [44](#), [395](#)
  - Magnetization Transfer, [20](#), [42](#), [265](#)
  - Magnetization Transfer Kinetics, [20](#), [43](#), [275](#)
  - Maximum Entropy Method Of Moments, [21](#), [44](#), [373](#)
  - Metabolic Analysis, [21](#), [43](#), [219](#)
  - Non-Linear Image Phasing, [21](#), [45](#), [405](#)
  - Polynomials
    - of Given Order, [21](#), [44](#)
    - of Unknown Order, [21](#), [44](#)
  - Test ASCII Model, [42](#)
  - Test Ascii Model, [20](#), [337](#)
  - Unknown Number of Exponentials, [20](#), [40](#), [143](#)
  - Unknown Polynomial Order, [293](#)
- Parameter File, [42](#)
- Number Of
  - Abscissa, [458](#)
  - Data Columns, [458](#)
  - Model Vectors, [458](#)
  - Priors, [458](#)
- Prior Probability, [459](#)
  - Amplitude, [460](#)
  - High, [459](#)
  - Low, [459](#)
  - Mean, [459](#)
  - NonLinear, [460](#)
  - Ordered, [460](#)
  - Parameter File, [459](#)
  - Peak, [459](#)
  - Prior Type, [460](#)
  - Standard Deviation, [459](#)
- Phase Cycling, [162](#)
- Plot Results Viewer, [71](#)
- Plots
  - Data and Model, [81](#)
  - Data, Model and Residuals, [81](#)
  - Expected Log Likelihood, [88](#)
  - Logarithm of the Posterior Probability, [91](#)
  - Maximum Entropy Histogram, [84](#)
  - Maximum Entropy Histograms, [83](#)
  - McMC Samples, [83](#), [85](#)
  - Parameter Vs Posterior Probability, [86](#), [87](#)

- Posterior Probability, [82](#)
- Posterior Probability Vs Parameter Value, [86](#)
- Residuals, [81](#)
- Scatter, [88](#), [91](#)
- png graphics, [59](#)
- Posterior Probability Vs Parameter Value, [86](#)
- Power Spectrum, [112](#), [123](#), [124](#)
- Prior Probabilities
  - Bayes Phase, [399](#)
  - Big Magnetization Transfer, [261](#)
  - Big Peak/Little Peak, [212](#)
  - Diffusion Tensor, [253](#)
  - Enter Ascii Model, [331](#), [333](#)
  - Errors In Variables, [306](#)
  - Magnetization Transfer, [269](#)
  - Magnetization Transfer Kinetics, [279](#)
  - Non-Linear Phasing Package
    - A, [408](#)
    - $\theta$ , [408](#)
- Prior Probability, [42](#), [65](#), [65](#)
  - Exponential, [67](#), [459](#)
  - Gaussian, [67](#), [104](#), [106](#), [459](#)
  - Jeffreys', [118](#)
  - Normalization Constant, [67](#)
  - Parameter, [68](#), [459](#)
  - Positive, [68](#), [460](#)
  - Uniform, [67](#), [103](#), [118](#), [459](#)
- Prior Viewer, [65](#), [93](#)
- Probabilities
  - Expected Log Likelihood, [453](#)
  - Likelihood, [453](#)
  - Posterior, [453](#)
  - Prior, [453](#)
- Product Rule, [99](#), [119](#), [344](#), [439](#)
- Referencing
  - Setting, [59](#)
- Reports
  - Accepted File, [76](#)
  - McMC Values File
    - General Description, [449](#)
    - Maximum Posterior Probability Simulations, [451](#)
    - Mean Values, [452](#)
    - Prior, [450](#)
    - Standard Deviations, [453](#)
- Restoring An Analysis, [22](#), [35](#), [40](#)
- ROI
  - Expanding, [63](#)
  - Pixels, [63](#)
  - Point, [62](#)
  - Polygon, [62](#)
  - Square, [62](#)
- Saving An Analysis, [35](#), [39](#)
- Schuster Periodogram, [112](#), [123](#)
- Screen Captures, [49](#)
- Settings
  - httpd server, [19](#)
- Software
  - Bayes Account, [29](#)
  - CC, [29](#)
  - Fortran, [29](#)
  - Installation, [29](#)
  - javaws, [29](#)
  - OS requirements, [29](#)
  - root requirements, [30](#)
- Start Up Window, [22](#), [33](#)
- Steepest Descents, [173](#)
- Subdirectories, [469](#)
  - Bayes, [39](#)
  - Bayes.model.fid, [470](#)
  - Bayes.Predefined.Spec, [469](#)
  - Bayes.test.data, [39](#)
  - BayesAnalyzeFiles, [470](#)
  - BayesAsciiModels, [93](#), [469](#)
  - BayesOtherAnalysis, [35](#), [73](#), [470](#)
  - fid, [36](#), [53](#)
  - images, [36](#), [38](#), [39](#), [59](#), [470](#)
  - model.compile, [470](#)
  - plugins, [470](#)
  - Properties, [470](#)
  - Resources, [470](#)
  - Spectroscopic
    - fid, [470](#)
  - Working Directories, [470](#)
- Subroutine Names, [464](#)
- Sufficient Statistics, [122](#)
  - Definition, [105](#)
  - Location Parameter, [108](#)
- Sum Rule, [100](#), [119](#), [344](#), [440](#)

- Test Ascii Model Package, **337**
  - Reports
    - Bayes Accepted, **339**
    - Mcmc Values, **339**
  - Using, **339, 428**
  - Viewers
    - Ascii Data, **337**
    - Fortran/C Models, **337**
    - Prior Probabilities, **337**
  - Widgets
    - Build, **337**
    - Find Outliers, **339**
    - System, **337**
    - User, **337**
- Thermodynamic Integration, **445, 449**
- Uninstall, **49**
- Unknown Number of Exponentials Package, **143**
  - Bayesian Calculations, **145**
  - Model Equation, **145**
  - Reports
    - Bayes Accepted, **143, 148**
    - Condensed, **148**
    - Console Log, **148, 149**
    - McMC Values, **148**
    - Prob Model, **148**
  - Using, **143**
  - Viewers
    - File, **148**
    - Plot Results, **149, 150**
    - Prior, **143**
    - Text, **148**
  - Widgets
    - Constant, **143**
    - Find Outliers, **143**
    - Order, **143**
- Unknown Polynomial Order Package, **293**
  - Bayesian Calculations, **295**
  - Files
    - Ascii, **293**
    - Bayes Analyze, **293**
    - Peak Pick, **293**
  - Model Equation, **295**
  - Number of data sets, **293**
  - Reports
    - Bayes Accepted, **293, 299**
    - Condensed, **299**
    - Console Log, **298, 299**
    - McMC Values, **299**
    - Polynomial Order Plot , **301**
    - Prob Model, **299**
  - Using, **293**
  - Viewers
    - File, **299**
    - Text, **299**
  - Widgets
    - Set Order, **293, 294**
    - Unknown Order, **293, 294**
- Viewers, **27, 52**
  - ASCII Data, **36**
  - Ascii Data, **27, 53, 56, 63, 137, 265, 275, 285, 293, 311, 329, 337, 341**
  - Expanding Plot, **53**
  - Printing, **53**
  - Right click, **53**
  - Bayes Model, **160**
  - Fid Data, **27, 265**
  - fid Data, **53, 53, 285, 293**
    - Auto Range, **59**
    - Autoscale, **56**
    - Clear Cursors, **56**
    - Clear Data, **57**
    - Copy, **59**
    - Cursor, **56**
    - Data Info, **57**
    - Expand, **56**
    - fn, **57**
    - Full, **56**
    - Get Peak, **56**
    - Phase Popup, **57**
    - Print, **59**
    - Properties, **59**
    - Referencing, **59**
    - Save As, **57, 59**
    - Set Preference, **57**
    - Units, **59**
    - Zoom, **59**
  - Fid Model, **27**
  - fid Model, **68, 186**
    - Build BA Model, **70, 159**
    - Data, **71**

- Horizontal, 71
- Model, 71
- Overlay, 71
- Report, 71
- Residual, 71
- Stacked, 71
- Trace, 71
- Vertical, 71
- File, 28, 80
- Fortran/C Models, 93, 330
- Image, 27, 59, 415
  - Autoset Grayscale, 61
  - Copy Selected, 62
  - Delete All, 61
  - Delete Selected, 61
  - Display Full, 61
  - Element Selection, 60
  - Export, 62
  - Get Statistics, 64, 65
  - Get Threshold Statistics, 65
  - Grayscale, 63
  - Image Selection, 60
  - List, 59
  - Load Selected Pixels, 61
  - Max, 64
  - Mean, 64
  - Min, 64
  - Right Click, 61
  - RMS, 64
  - Save Displayed, 62
  - Save Statistics, 65
  - Sdev, 64
  - Set Image Area, 62
  - Show Histogram, 61
  - Show Info, 62
  - Slice, 62
  - Slice Selection, 60
  - Statistics, 60
  - Value, 64
  - View Selected Pixels, 61
  - Viewer Settings, 62
  - Viewing, 62
  - X Pos, 64
  - Y Pos, 64
- Plot Results, 28, 71
- Prior, 27, 65
  - Prior Probabilities, 138, 312
  - Text, 141, 271, 281, 290, 309, 322, 335, 353
  - Text Results, 26, 28, 52, 74
    - Bayes Analyze, 176
- Widgets
  - Analyze Image Pixel Package
    - Build, 411
    - Find Outliers, 411
    - Get Statistics, 413
    - System, 411
    - User, 411
  - Analyze Image Pixel Unique Package
    - Build, 423
    - Find Outliers, 423
    - Get Statistics, 425
    - System, 423
    - User, 423
  - Ascii Data Viewer
    - Delete, 53
    - Left-mouse, 53
    - Right-mouse, 53
  - Bayes Analyze Package
    - By, 158, 176
    - First Point, 163
    - From, 158, 176
    - Imag Offset, 163
    - Mark, 159
    - Max New Res, 157
    - New, 159
    - Noise, 158
    - Phase, 157
    - Primary, 158
    - Real Offset, 163
    - Remove, 159
    - Remove All, 159
    - Reset, 159, 193
    - Restore, 159
    - Save, 159
    - Secondary, 159
    - Shim Order, 157, 163
    - Signal, 158
    - To, 158, 176
  - Bayes Find Resonances Package
    - Build FID Model, 240, 241, 246
    - Constant, 239, 242

- First Trace, 239
- Last Trace, 239
- Model Fid Number, 241
- Phase Model, 239, 242
- Bayes Metabolite Package
  - Fid Model, 221
  - Fid Model Viewer, 221
  - Load System Metabolite File, 219
  - Load System Resonance File, 221
  - Load User Metabolite File, 219
  - Load User Resonance File, 221
  - Shift Left, 221, 222
  - Shift Right, 221, 222
- Bayes Test Data Package
  - # Images, 427
  - # Slices, 427
  - Abscissa, 427
  - ArrayDim, 427
  - Build, 427
  - Get Job, 428
  - Max Value, 427
  - Noise SD, 427
  - Pe, 427
  - Ro, 427
  - Run, 428
  - Set (server), 428
  - Status, 428
  - System, 427
  - User, 427
- Big Magnetization Transfer Package
  - Find Outliers, 259
- Big Peak/Little Peak Package
  - Metabolite, 207
  - Solvent, 207
- Diffusion Tensor Package
  - Abscissa Options, 248
  - Find Outliers, 247
  - Include Constant, 247, 248, 255
  - Tensor Number, 247, 248, 255
  - Use b Matrix, 255
  - Use b Vectors, 254, 255
  - Use g Vectors, 254
- Enter Ascii Model Package
  - Find Outliers, 329
  - System, 329
  - User, 329
- Enter Ascii Model Selection Package
  - Find Outliers, 341
  - System, 341
  - User, 341
- Errors In Variables Package
  - Given Errors In, 303
  - Order, 303
- Fid Data Viewer
  - Autoscale, 56
  - Clear Cursors, 56
  - Cursor A, 56
  - Cursor B, 56
  - Delta, 56
  - Display Type, 56
  - Expand, 56
  - Full, 56
  - Get Peak, 56
  - Left-mouse, 56
  - Options, 57, 59
  - Right-mouse, 56
  - Trace, 70
- Fortran/C Model Viewer
  - Abscissa Spinner, 93
  - Add Prior, 96
  - Allow/Disallow Editing, 97
  - Cancel and Exit, 96
  - Changing Models, 94
  - Code, 93, 94
  - Compile Results, 97
  - Compiling, 96
  - Create/Edit Model, 93
  - Data Columns Spinner, 93
  - Derived, 96
  - Edit/Create New Model, 93, 94
  - High, 97
  - Low, 97
  - Mean, 97
  - Model, 96
  - Model Vectors, 93
  - Name (parameter), 97
  - Order, 97
  - Parameter Type, 97
  - Parameters button, 93, 94, 96
  - Prior Type, 97
  - Priors, 96
  - Remove All (priors), 96

- Remove Prior, 96
- Remove Selected Model, 93
- Save and Load, 96
- Standard Deviation, 97
- Given Exponential Package
  - Constant, 137, 139
  - Find Outliers, 137
  - Order, 137, 139
- Given Polynomial Order Package
  - Set Order, 285
- Global
  - Bayes Find Outliers, 27
  - Cancel, 26, 51
  - Edit Servers, 26
  - Get Job, 26, 51, 137, 143, 151, 155, 209, 221, 241, 247, 259, 267, 277, 285, 293, 305, 311, 331, 339, 343, 357, 364, 375, 413, 417, 425, 428
  - Reset, 27
  - Restore Analysis, 22
  - Run, 26, 51, 137, 143, 151, 155, 207, 221, 241, 247, 248, 259, 267, 277, 285, 293, 305, 311, 329, 337, 343, 357, 364, 373, 413, 415, 425, 428
  - Save, 27
  - Set (server), 26, 52, 137, 143, 151, 155, 207, 221, 239, 247, 259, 265, 277, 285, 293, 305, 311, 329, 337, 343, 355, 364, 373, 413, 415, 425, 428
  - Status, 26, 52, 137, 143, 151, 155, 207, 221, 241, 247, 259, 267, 277, 285, 293, 305, 311, 329, 337, 343, 355, 364, 373, 413, 415, 425, 428
- Image Model Selection Package
  - System, 415
  - User, 415
- Image Viewer
  - Element Number, 62
  - Get Statistics, 64
  - Get Threshold Statistics, 65
  - Grayscale, 63
  - Save Statistics, 65
  - Slice Number, 62
  - Value, 64
  - X Pos, 64
  - Y Pos, 64
- Inversion Recovery Package
  - Find Outliers, 151
- Kernel Density Function Package
  - Kernel Type, 364
  - Output Size, 364
- Linear Phasing Package
  - cf, 403
  - Display, 403
  - Display Array Element, 403
  - fn, 403
  - fn1, 403
  - Image Type, 402
  - Load An Image, 402
  - np, 403
  - nv, 403
  - Process, 403
- Magnetization Transfer Kinetics Package
  - Load, 275, 281
  - Set, 275
  - Uncertainty, 275
- Magnetization Transfer Package
  - Find Outliers, 265
- MaxEnt Density Function Estimation Package
  - Histogram Size, 373
  - Order, 373
- Non-Linear Phasing Package
  - Process, 409
  - Write Ascii images, 409
  - Write imaginary images, 409
- Prior Viewer
  - High, 65
  - Low, 65
  - Mean, 65
  - Prior Type, 67
- Server
  - Edit, 52
  - Name, 26, 52, 52
  - Set (server), 48
  - Setup, 48, 52
- Test Ascii Model Package
  - Find Outliers, 339
  - System, 337
  - User, 337
- Text Results Viewer
  - Copy, 74

- Down arrow, [74](#)
- Enable Editing, [74](#)
- Print, [74](#)
- Save (a copy), [74](#)
- Save As, [74](#)
- Settings, [74](#)
- Up arrow, [74](#)
- Unknown Number of Exponentials Package
  - Constant, [143](#)
  - Find Outliers, [143](#)
  - Order, [143](#)
- Unknown Polynomial Order Package
  - Set Order, [293](#), [294](#)
  - Unknown Order, [293](#), [294](#)
- WorkDir
  - Creating, [22](#), [33](#), [46](#)
  - Deleting, [22](#), [33](#), [46](#)
  - List, [24](#), [46](#)
  - Loading, [46](#)
  - Name, [46](#)
  - Popup, [47](#)