

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

September 18, 2018

Chapter 13

Big Magnetization Transfer

The Big magnetization transfer package analyzes data where two sites are exchanging magnetization under the assumption that one of the sites is essentially infinite compared to the other. Consequently, the big site is essentially unchanging and the solution for the other site simplifies, Eq. (13.1) below. The interface to this package is shown in Fig. 13.1. To use this package, you must do the following:

Select the Big Magnetization Transfer package from the Package menu.

Load one or more Ascii data sets using the Files menu. When the data have been successfully loaded, the data are displayed in the Ascii Data viewer.

Check the Analysis Options/Find Outliers box if you suspect outliers are present in the data.

Review the prior probabilities for the K_d , R_d and R_w parameters using the Prior Viewer.

Select the server that is to process the analysis.

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 the analysis on the selected server by activating the Run button.

Get the 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.

13.1 The Bayesian Calculation

The Big magnetization transfer problem is one in which a very large spin reservoir is exchanging magnetization with a much smaller spin reservoir. We will call the larger reservoir the Solvent, and the other the Small reservoir or resonance. When one reservoir is much greater than the other, the

Figure 13.1: The Big Magnetization Package Interface

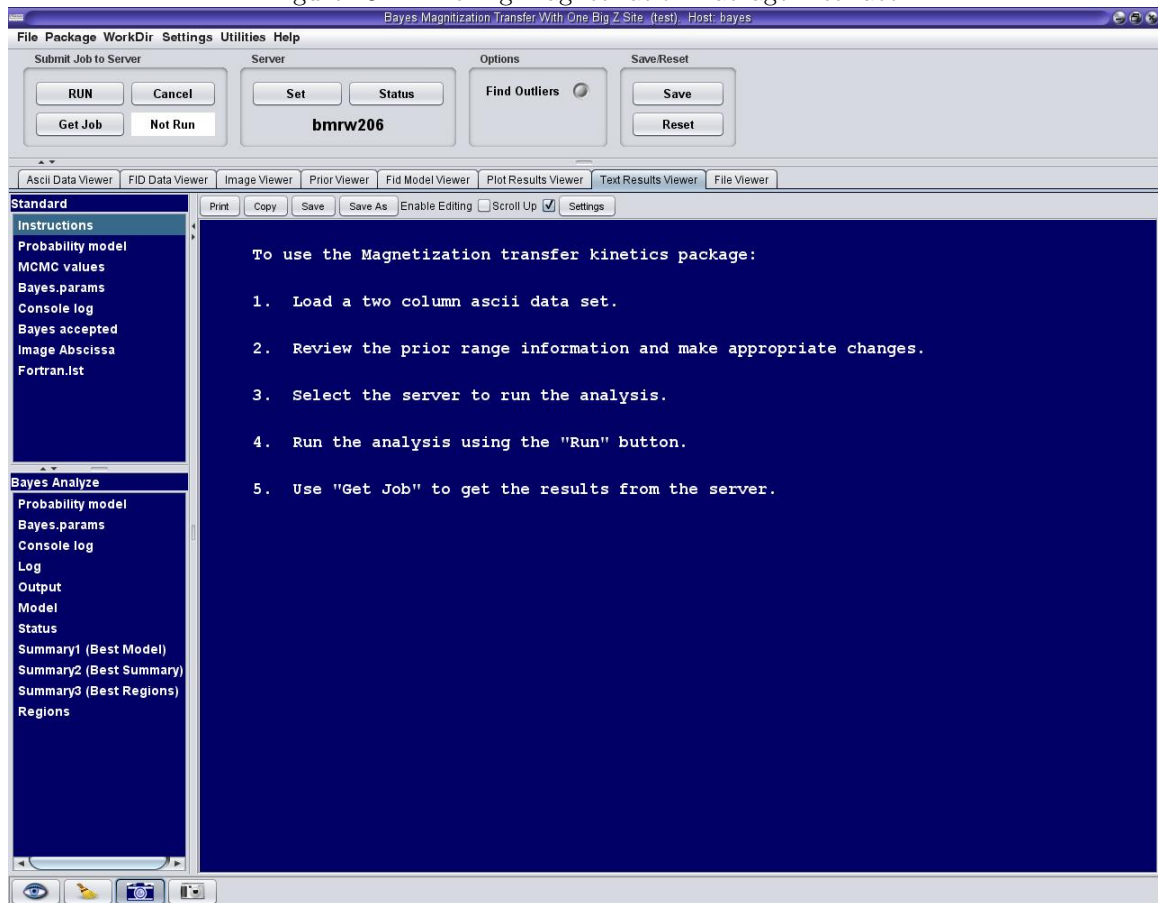


Figure 13.1: The interface to the Big Magnetization Transfer Package is shown here. The Big magnetization transfer interface allows you to analyze magnetization transfer data where one of the two sites may be considered as infinite compared to the other, see text for details.

Solvent is unaffected by the the transfer of magnetization to or from Small reservoir. Consequently, the solution to magnetization exchange equations simplify, one obtains

$$M_d(t) = M_{z0} \left(1 - \frac{2K_d}{R_w - K_d - R_d} \left[e^{-(R_d+K_d)t_i} - e^{-R_w t_i} \right] \right) \quad (13.1)$$

where M_{z0} is the initial Small reservoir magnetization, K_d is the rate at which the Small reservoir is exchanging magnetization to the Solvent, R_w is the inverse of the T_2 time for Solvent reservoir, R_d is the R_2 relaxation rate of the Small reservoir and this equation implicitly assumes that the magnetization is fully inverted.

Markov chain Monte Carlo is used to draw samples from the joint posterior probability for all of the parameters. Form these samples, the marginal posterior probability for each parameter is computed. For example the posterior probability for the exchange rate K_d is computed as

$$P(K_d|DI) = \int P(K_d M_{z0} R_w R_d \sigma | DI) dM_{z0} dR_w dR_d d\sigma \quad (13.2)$$

where all of the parameters except the parameter of interest have been removed by marginalization. The joint posterior probability for the parameters, the integrand of this equation, is factored using Bayes' theorem and the product rule to become

$$P(K_d M_{z0} R_w R_d \sigma | DI) \propto P(K_d M_{z0} R_w R_d \sigma | I) P(D | K_d M_{z0} R_w R_d \sigma I) \quad (13.3)$$

where $P(K_d M_{z0} R_w R_d \sigma | I)$ is the joint prior probability for the parameters and $P(D | K_d M_{z0} R_w R_d \sigma I)$ is the likelihood. The joint prior probability or the parameters is factored into independent prior probabilities for each of the parameters separately

$$P(K_d M_{z0} R_w R_d \sigma | I) = P(K_d | I) P(M_{z0} | I) P(R_w | I) P(R_d | I) P(\sigma | I). \quad (13.4)$$

The prior probability for the standard deviation of the noise prior probability, $P(\sigma | I)$, is assigned a Jeffreys' prior, $P(\sigma | I) \propto 1/\sigma$. The prior probability for the amplitude $P(M_{z0} | I)$, was assigned using a using a very broad unbounded Gaussian of zero mean having a standard deviation of 3×10^5 . The remaining three prior probabilities, $P(K_d | I)$, $P(R_w | I)$ and $P(R_d | I)$ all default to a prior positive. However, these priors are under user control and they may changed by the user. The likelihood, $P(D | K_d M_{z0} R_w R_d \sigma I)$ was assigned using a Gaussian prior probability having standard deviation σ . If we now collect all of the priors, assign the likelihood, and evaluate the integrals over both M_{z0} and σ , one obtains:

$$P(K_d M_{z0} R_w R_d \sigma | DI) \propto P(K_d | I) P(R_w | I) P(R_d | I) \left[N \overline{d^2} - \overline{h^2} \right]^{-\frac{N}{2}} \quad (13.5)$$

where $\overline{d^2}$ is the mean-square data value and is given by

$$\overline{d^2} = \frac{1}{N} \sum_{i=1}^N d_i^2. \quad (13.6)$$

The sufficient statistic, $\overline{h^2}$, is given by

$$\overline{h^2} = \frac{T^2}{g} \quad (13.7)$$

where T is the projection of the data onto the model and is given by

$$T = \sum_{i=1}^N d_i \left(1 - \frac{2K_d}{R_w - K_d - R_d} \left[e^{-(R_d+K_d)t_i} - e^{-R_w t_i} \right] \right) \quad (13.8)$$

and g is the squared length of the model:

$$g = \sum_{i=1}^N \left(1 - \frac{2K_d}{R_w - K_d - R_d} \left[e^{-(R_d+K_d)t_i} - e^{-R_w t_i} \right] \right)^2. \quad (13.9)$$

It is Eq. (13.5) that is targeted by the Markov chain Monte Carlo simulations using simulated annealing. Note that this posterior probability does not contain the initial magnetization. However, in the process of computing this quantity the maximum posterior probability estimate of this parameter is computed and output for each value of the exchange and relaxation rates. While not strictly the Bayesian estimate of this parameter, the distribution of these estimates provide good mean and standard deviation estimates of the initial magnetization.

13.2 Outputs From The Big Magnetization Transfer Package

The Big Magnetization Transfer Package is an example of a preloaded Enter Ascii model. Preloaded means that when the Big Magnetization Transfer package is selected, the interface copies an Ascii model, MtZBig.f, from the system directory into the current experiment and starts up the Enter Ascii package. Consequently, the outputs from this package are all Enter Ascii outputs. The Text outputs files from the Big Magnetization Transfer packages consist of: “Bayes.prob.model,” “BayesEnterAscii.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 decay rate constants, decay times, the amplitudes for each data set for each exponential

The full spectrum of data typical of this experiment is shown in Fig. 13.2. Note the presence of a water suppression artifact near 5ppm. To acquire this data one typically inverts the water, suppresses it, and finally acquires the Fid. The resonance exchanging magnetization with the water is the small resonances located at 11ppm. If we expand this region and then do a horizontal display, one obtains the spectra shown in Fig. 13.3. The Solvent resonance begins at its equilibrium value. When the Solvent resonances is inverted, negative magnetization flows into the Small reservoir bring its value down. At different delay times, different amounts of negative magnetization exchange with the Solvent resonance affecting its intensity in a predictable manner. The peak heights or amplitudes as determined by Bayes Analyze are used as input to the analysis. An example of data using a peak pick is shown in Fig. 13.3. Note that the Solvent resonance was inverted, as the Solvent exchanges negative magnetization with the Small resonance, the Small resonance is eventually pulled down. As the delay time increases the Small resonance has time to relax back toward equilibrium and eventually recovers.

Figure 13.2: Big Magnetization Transfer Example Fid

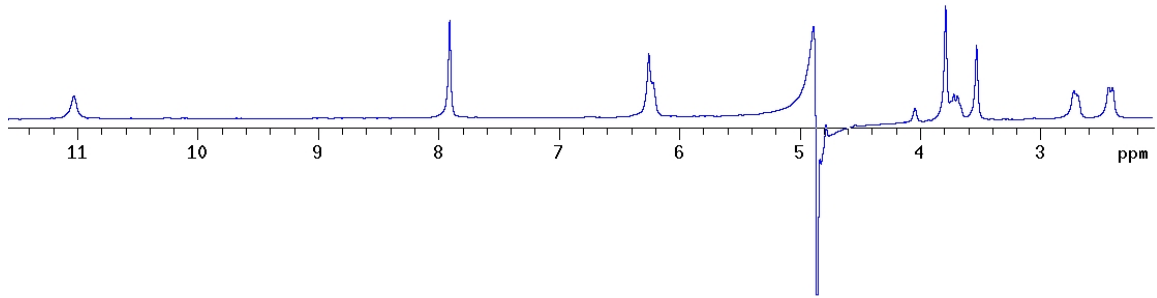


Figure 13.2: The full spectrum of the Fid data used in the big magnetization analysis. Note the water suppression artifact near 5ppm. The peak exchanging magnetization with the water is the small resonance near 11ppm.

Figure 13.3: Big Magnetization Transfer Expansion

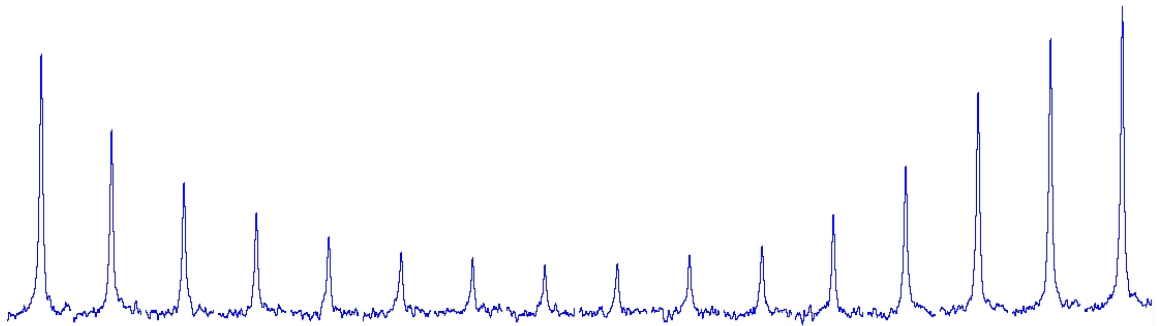


Figure 13.3: The peak exchanging magnetization begins at its equilibrium value. When the Solvent is inverted, negative magnetization flows into the Small reservoir bringing this reservoir down. At different delay times the Solvent is more fully relaxed and the Small resonance begins to recover, until at the longest delay time the Small resonance has returned to equilibrium. It is the amplitudes of the Small resonance that serve as input to this analysis.

Figure 13.4: Big Magnetization Transfer Peak Pick

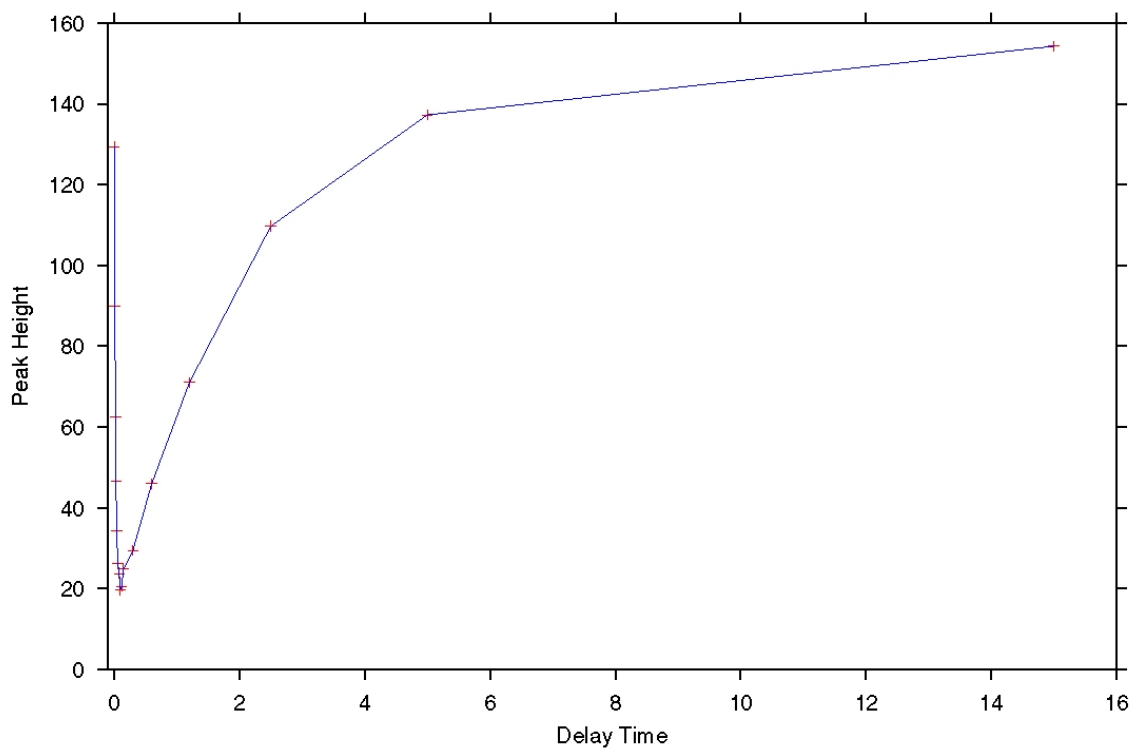


Figure 13.4: The peak heights or amplitudes (as determined by Bayes Analyze) serve as input to the Big magnetization transfer package. Here the peak heights for the spectra shown in Fig. 13.3 were used as input to the analysis. Note the Solvent magnetization starts fully relaxed, then after the Solvent is inverted, the negative Solvent magnetization begins to bring the Small reservoir down. As a function of delay time this continues for a while and then eventually the Small resonance recovers back to equilibrium.

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}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 ^2H and ^{13}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}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}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
- λ_ℓ 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](#)
 - Procparr, [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
 - Δ , [254](#)
 - Γ , [254](#)
 - δ , [254](#)
 - σ , [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](#)
 - θ , [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, 373, 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](#)