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 1

Given Exponential Model

The Given Exponential Package estimates amplitudes and decay rate constants in data that are known to contain signals which are sums of exponentials. This signal may or may not contain a constant offset, and the number of exponentials in the data need not be known. The calculations presented in this Chapter describe the given model, i.e., given the number of exponentials and whether a constant is or is not present. We describe the calculations for the unknown number of exponentials in Chapter 6. The input data files analyzed by this package are Ascii and may be input from Ascii files, a peak pick, a Bayes Analyze file or they may be loaded from an image pixel. When "Exponential" package button is activated, the interface window shown in Fig. 1.1 is displayed. This is the interface for both "Given" and "Unknown" number of exponentials. To use this package, you must do the following:

Select the exponential package from the Package menu.

Load one or more Ascii data sets using the Files menu. When a data set is successfully loaded the data is plotted in the Ascii Data viewer.

Set the number of exponentials in the model using the Model/Order selection menu.

Check the Model/Constant box if the data contains an offset.

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

Review the prior probabilities for the decay rate constant using the Prior Viewer.

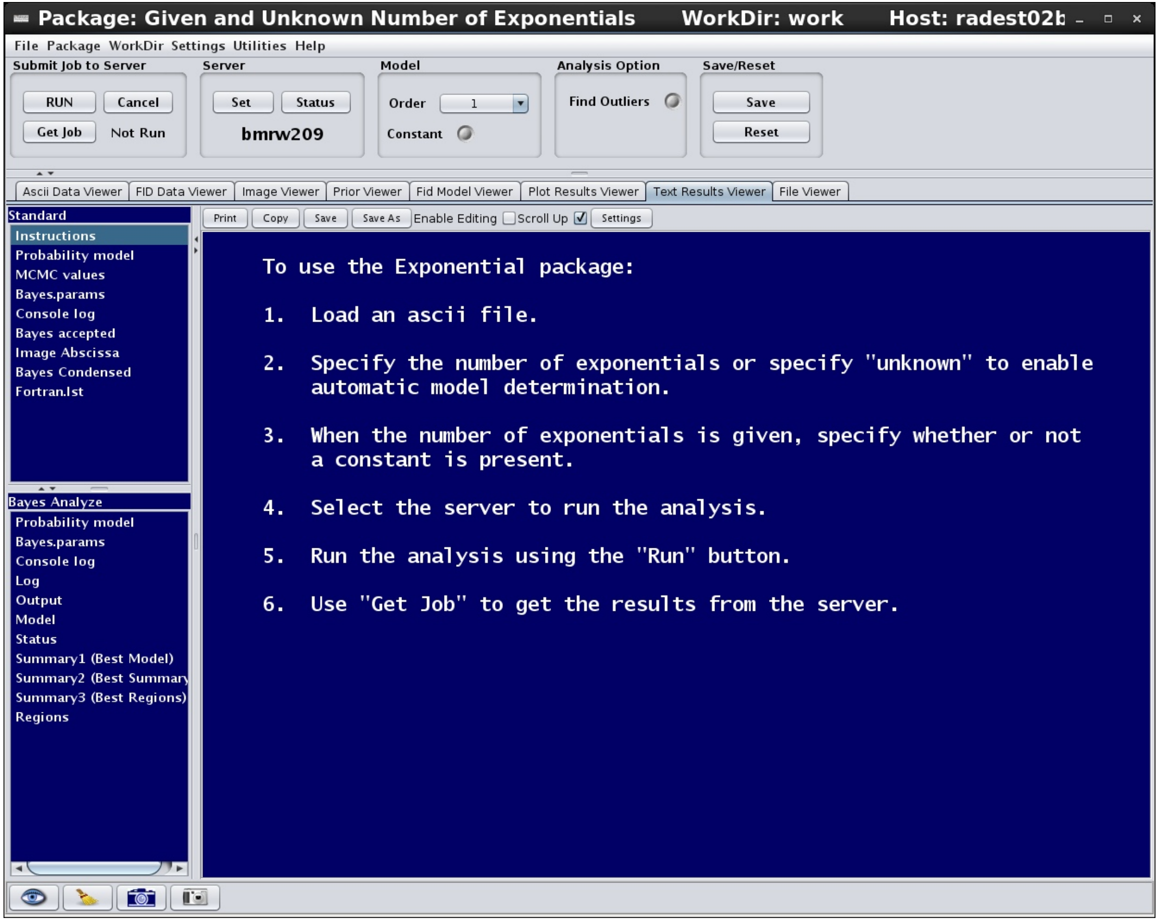
Select the server that is to process the analysis.

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.

Figure 1.1: The Given And Unknown Number Of Exponential Package Interface



```
To use the Exponential package:

1.  Load an ascii file.

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

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

4.  Select the server to run the analysis.

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

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

Figure 1.1: When the Exponential package is selected, this is the displayed interface. The package setup widgets, in this case labeled "Model," allow you to select the number of exponentials in the data and they allow you to specify whether or not a constant offset is present. Additionally, the prior viewer can be used to set the prior probability for the decay rate constants. Note in this package the posterior probabilities are marginal posterior probabilities, so there are no adjustable prior probabilities for the amplitudes.

1.1 The Bayesian Calculation

The sums of exponential package process data that are known to contain exponential signals of the form:

$$d_{ik} = C_k + \sum_{j=1}^{m} A_{jk} \exp\{-\alpha_j t_{ik}\} + n_{ik} \tag{1.1}$$

where d_{ik} is the ith data value in the kth data set, C_k is the constant offset in the kth data set, m is the number of exponentials, A_{jk} is the amplitude or intensity of the jth exponential in the kth data set, α_j is the jth exponential decay rate constant, t_{ik} is the ith abscissa value in the kth data set, and as this equation implies, the abscissa values and the sampling times need not be the same from one data set to the next. In Fig. 1.1, the model widgets, allow you to set the number of exponentials and allow you to indicate if a constant is present. Additionally, the prior viewer can be used to set the prior probability for the decay rate constants. Finally, the number of data sets n is determined by the number of Ascii data sets loaded into the analysis. If 5 Ascii data sets are loaded, the $n = 5$.

When the number of exponentials are given, the problem is one of parameter estimation and the program that implements this Bayesian calculation computes the marginal posterior probability for each of the parameters appearing in the model. For example, the marginal posterior probability for the decay rate constant, α_j, is computed from the joint posterior probability for all of the parameters using the sum rule:

$$P(\alpha_j|DI) = \int d\{A\}d\{C\}d\{\sigma\}d\alpha_1 \ldots d\alpha_{j-1}d\alpha_{j+1} \ldots d\alpha_m P(\{A\}\{C\}\{\sigma\}\{\alpha\}|DI) \tag{1.2}$$

where the integral is over all of the parameters except the parameter of interest, in this case α_j. The notation, $\{\cdot\}$ is being used to stand for all of the enclosed quantities. So for example if there are three exponentials and 5 data sets, there are 15 total amplitudes represented by $\{A\}$. Similarly, because there is one constant per data set, then there would be 5 total constants represented by $\{C\}$. The right-hand side of this equation was factored using the rules of probability theory and Bayes Theorems' [1]

$$\begin{aligned} P(\{A\}\{C\}\{\sigma\}\{\alpha\}|DI) \quad \propto \quad & \left[\prod_{l=1}^{m} P(\alpha_l|I)\right] \\ \times \quad & \left[\prod_{k=1}^{n} P(C_k|I)P(\sigma_k|I)\right] \\ \times \quad & \left[\prod_{k=1}^{n}\prod_{j=1}^{m} P(A_{jk}|I)\right] \\ \times \quad & \left[\prod_{k=1}^{n} P(D_k|\{A\}_k\{\alpha\}C_k\sigma_k I)\right] \end{aligned} \tag{1.3}$$

where m is the given number of exponentials, n is the number of data sets, $P(\alpha_l|I)$ is the prior probability for the lth decay rate constants, $P(C_k|I)$ is the prior probability for the constant in the kth data set, $P(\sigma_k|I)$ is the prior probability for the standard deviation of the noise, $P(A_{jk}|I)$ is the prior probability for the amplitudes of the jth exponential in the kth data set, and $P(D_k|\{A\}_k\{\alpha\}C_k\sigma_k I)$

is the direct probability or likelihood of data set D_k given the amplitudes, $\{A\}_k$, in the kth data set, the constant offset, C_k, and the standard deviation of the noise, σ_k.

The various probabilities are assigned as follows The prior probability for the decay rate constant, $P(\alpha_l|I)$ are user defined and the functional form of this prior probability can be any of the following: a uniform prior probability, a bounded Gaussian, an exponential prior probability or a prior positive. When the interface initializes the exponential package, a default prior probability for the decay rate constant is defined using the maximum value of the abscissa. This default prior probability is a bounded Gaussian prior probability that goes through 4.5 e-foldings over the decay rate constant ranges shown in the interface. If the maximum decay rate constant is $\alpha_{\rm Max}$, then the default prior probability for the decay rate constant is given by

$$P(\alpha_l|I) = \begin{cases} \dfrac{1}{N_l}\exp\{-\dfrac{\alpha_l^2}{2\sigma_l^2}\} & \text{if } (0 \le \alpha_l \le \alpha_{\rm Max}) \\ 0 & \text{otherwise} \end{cases} \tag{1.4}$$

where N_l is a normalization constant. If we make the assumption that the exponential signal components decay to no more than 20 e-foldings over the run of the data, then we can define a maximum decay rate constant:

$$\alpha_{\rm Max} T_{\rm Max} \equiv 20, \tag{1.5}$$

$T_{\rm Max}$ is the maximum abscissa value, so

$$\alpha_{\rm Max} = \frac{20}{T_{\rm Max}}, \tag{1.6}$$

and σ_l is set so that the prior goes through 4.5 e-foldings:

$$\frac{(\alpha_{\rm Max})^2}{2\sigma_l^2} = 4.5. \tag{1.7}$$

Consequently,

$$\sigma_l \approx \frac{6.666666}{T_{\rm Max}}. \tag{1.8}$$

The user assigns only a single prior probability for the decay rate constants and the interface uses this prior for all decay rate constants.

The prior probabilities for the amplitudes, the $P(A_{jk}|I)$, are assigned using broad Gaussian that range from $-\infty$ to $+\infty$,

$$P(A_{jk}|I) = \left(\frac{2\pi\sigma_k^2}{\delta^2}\right)^{-\frac{1}{2}} \exp\left\{-\frac{\delta^2}{2\sigma_k^2}A_{jk}^2\right\} \tag{1.9}$$

where $\delta = 0.01$ in the given and unknown number of exponentials. In these package you cannot change the prior probability for the amplitudes. Similarly, the prior probability for the constant offset in each data set, $P(C_k|I)$, is also assigned as a Gaussian prior probability using

$$P(C_k|I) = \left(\frac{2\pi\sigma_k^2}{\delta^2}\right)^{-\frac{1}{2}} \exp\left\{-\frac{\delta^2}{2\sigma_k^2}C_k^2\right\} \tag{1.10}$$

the same functional form with δ also equal to 0.01. Consequently, it is possible for this package to estimate either the amplitudes or the constant offsets to be negative when the prior information available to the user would constrain it to be positive. If this is unacceptable, in the Enter Ascii Model package there is a full suite of exponential models that allow you to control the prior range on the amplitudes as well as the decay rate constants, Chapter 20. The prior probability for the standard deviation of the noise, the σ_k, were assigned using Jeffreys' priors [33],

$$P(\sigma_k|I) \propto \frac{1}{\sigma_k}. \tag{1.11}$$

Finally, the direct probability for the data was assigned using a Gaussian likelihood function. This Gaussian had a standard deviation given by σ_k that is specific to each data set.

The exponential model equation, Eq. (1.1) is symmetric under relabeling of the amplitudes and decay rate constants. This symmetry causes the joint posterior probability for the decay rate constants to be symmetric in the sense that if there is a peak at $\alpha_1 = \beta$ and $\alpha_2 = \gamma$, then there is also a peak at $\alpha_1 = \gamma$ and $\alpha_2 = \beta$; this symmetry is caused because the model does not tell us which exponential signal corresponds to to which model component. Consequently, a convention must be introduced which brakes this symmetry. In the calculations implemented here, we break this symmetry by ordering the rate constants: $\{\alpha_1 < \alpha_2 < \alpha_3, \text{etc.}\}$.

The full Bayesian calculation and the assignment of the prior probabilities is discussed in reference [15] and this paper is available in pdf by activating this link. Additionally, much more about exponential parameter estimation is contained in [16, 17]. The first paper describes the problem of determining the number of exponentials in a given sample of data, while the second paper discusses how the accuracy of the parameter estimates depends on the number of data values, signal-to-noise level and the rate of decay of the sample.

1.2 Outputs From The Given Exponential Package

The Text outputs files from the exponential packages consist of: "Bayes.prob.model," "BayesExpGiven.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 and finally there are probability density functions for the standard deviation of the noise in each data set.

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 f¨r 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 13C 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}H 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 13C 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
  Procpar, 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
    - procpar, 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
  - procpar, 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, 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