

Bayesian Data-Analysis Toolbox
Release 4.23, Manual Version 3

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Chapter 16

Given Polynomial Order

The Given polynomial Order package fits polynomials to two column Ascii data when the order of the polynomial is known. The interface to the Given Polynomial Order package is shown in Figure 16.1. This interface differs from most others in one respect, there are no parameter ranges to enter, so use of the interface is particularly simple. To use this package, you must do the following:

Select the Polynomial Models package from the Package menu. When selected this menu will bring up the “Given” and “Unknown” polynomial model interface.

Load one two column Ascii data sets. The data may be loaded using the Files menu. You can also load an arrayed Fid and then use a single cursor to mark the center of a peak and use the “Get Peak” button on the bottom right of the Fid viewer. Finally, the “Files/Load Ascii/Bayes Analyze” button can be used to load an Ascii data set from the amplitudes estimated by Bayes Analyze. When a data set is successfully loaded the data is plotted in the Ascii Data viewer. This package does not allow you to run with multiple data sets. If you attempt to do so, you will be prompted to remove all but a single file.

Set the Polynomial order using the “Set Order” selection widget. For the Given Polynomial Order, the order can be from 1 to 55.

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 16.1: Given Polynomial Order Package Interface

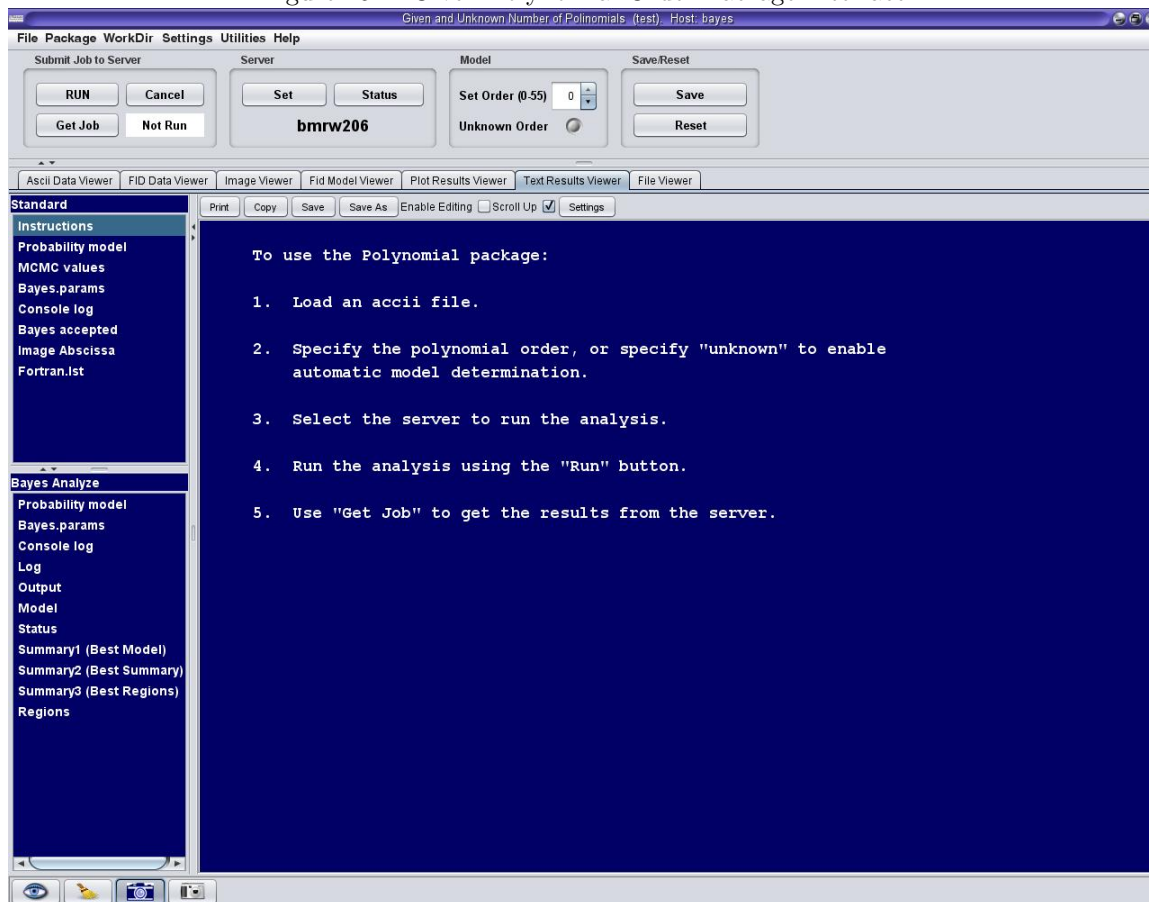


Figure 16.1: This panel is interface to the Given Polynomial Order package. Because of the way this calculation is done very high orders are possible and numerically stable. However, the high orders, above 40, require very high signal-to-noise and even then roundoff errors degrade the accuracy to 4 or 5 decimal places.

16.1 The Bayesian Calculation

The polynomial model is just that, its a model in which a polynomial is fit to the data:

$$d_i = \sum_{j=0}^m A_j G_j(t_i) + n_i \quad (16.1)$$

with

$$G_j(t_i) = t_i^j \quad (16.2)$$

where A_j is the amplitude of the j th polynomial, n_i represents noise in the i th data value and we have written these polynomials as $G_j(t_i)$ for notational convenience. We will think of these polynomials as functions of time, but in the analysis which follows t is simply a single column abscissa and may be any quantity. In the problem we are describing here, m is the given order of the polynomial. Additionally, the assumption that these are polynomials is unimportant in the following discussions, the $G_j(t_i)$ could be any set of functions.

16.1.1 Gram-Schmidt

The Bayesian calculation is implemented using Markov chain Monte Carlo with simulated annealing to draw samples for the joint posterior probability for the parameters. Before we do this calculation we introduce a change of function and a change of variables. The reason for this is simply that computing polynomials of the form $\sum_{j=0}^m A_j t_i^j$ is computationally vary unstable in the sense that only orders up to about 8 can be computed using single precision arithmetic. You can get to higher orders only by using numerical procedures that avoid differencing large numbers, for example the remainder theorem. However, here we take a different approach by transforming the problem to something that is computationally more stable. Using Gram-Schmidt, the polynomials are transformed to a set of orthogonal polynomials. We then solve the problem using these orthogonal polynomials and finally, we transform the derived amplitudes back to the A_j given in Eq. (16.1). If we designate the Gram-Schmidt polynomials as $H_j(t_i)$ and the expansion coefficients as B_j , Eq. (16.1) becomes:

$$d_i = \sum_{j=0}^m B_j H_j(t_i) + n_i. \quad (16.3)$$

We chose the Gram-Schmidt polynomials because they can be computed trivially from the t_i^j , they preserve the notation of the order of the polynomial, and each polynomial depends only on the lower orders, not the higher orders. This change of variables and change of function is an identity, i.e., the polynomial expansions in Eq. (16.1) and Eq. (16.3) are exactly equal to each other. Finally, the amplitudes, B_j and A_j , are linearly related to each other through an lower triangular matrix, and consequently, the conversion back and forth between these representations is very easy to program.

As a reminder to those unfamiliar with Gram-Schmidt polynomials, the normalized Gram-Schmidt polynomials $H_j(t_i)$, are generated recursively from the $G_j(t_i)$ using:

$$H_j(t_i) = \frac{1}{C_{jj}} \left[G_j(t_i) - \sum_{\ell=0}^{j-1} C_{j\ell} H_\ell(t_i) \right] \quad (16.4)$$

where the sum is not present for the first polynomial, and

$$C_{j\ell} = \sum_{i=1}^N G_j(t_i) H_\ell(t_i) \quad (0 \leq j \leq \ell). \quad (16.5)$$

Gram-Schmidt polynomials have the property

$$\sum_{i=1}^N H_j(t_i) H_\ell(t_i) = \delta_{j\ell} \quad (16.6)$$

where $\delta_{j\ell}$ is zero if $j \neq \ell$ and one if $j = \ell$.

To derive the relationship between the A_j and the B_j , note that the expansions given by Eq. (16.1) and Eq. (16.3) are identities, so can write

$$\sum_{k=0}^m A_k G_k(t_i) = \sum_{j=0}^m B_j H_j(t_i) \quad (16.7)$$

where we changed the summation index on the left-hand side just to remind people that these summations are independent of each other. Multiplying this equation by $H_\ell(t_i)$, and summing over time:

$$\sum_{i=1}^N \sum_{k=0}^m A_k G_k(t_i) H_\ell(t_i) = \sum_{i=1}^N \sum_{j=0}^m B_j H_j(t_i) H_\ell(t_i). \quad (16.8)$$

The right-hand side of this equating is zero unless $j = \ell$ and then one obtains

$$\sum_{i=1}^N \sum_{k=0}^m A_k G_k(t_i) H_\ell(t_i) = B_\ell \quad (16.9)$$

and the sum over time on the left-hand side of this equation can be written as

$$\sum_{k=0}^m A_k \left[\sum_{i=1}^N G_k(t_i) H_\ell(t_i) \right] = B_\ell. \quad (16.10)$$

The quantity in big square brackets is just the right-hand side of Eq. (16.5), so this equation becomes

$$\sum_{k=0}^m A_k C_{k\ell} = B_\ell. \quad (16.11)$$

The matrix $C_{k\ell}$ is a lower triangular matrix, so inverting it is trivial and one can use this equation solve for the nonorthogonal expansion coefficients, the A_k , from the orthogonal expansion coefficients, the B_j .

16.1.2 The Bayesian Calculation

The Bayesian calculation is for the joint posterior probability for the amplitudes, B_j , given the data and the prior information. This joint probability, denoted by $P(B_0 B_1 \dots B_m | DI)$, is computed by application of Bayes' theorem

$$P(B_0 B_1 \dots B_m | DI) \propto P(B_0 B_1 \dots B_m | I) P(D | B_0 B_1 \dots B_m I) \quad (16.12)$$

where $P(B_0B_1 \dots B_m|I)$ is the joint prior probability for the amplitudes, and $P(D|B_0B_1 \dots B_mI)$ is the likelihood. Because each polynomial is orthogonal, we will factor the joint prior probability for the amplitudes, $P(B_0B_1 \dots B_m|I)$, into a series of independent prior probabilities:

$$P(B_0B_1 \dots B_m|I) = \prod_{j=0}^m P(B_j|I) \quad (16.13)$$

and each of the $P(B_j|I)$ will be assigned a unbound Gaussian. The posterior probability for the B_j , is thus given by:

$$P(B_0B_1 \dots B_m|DI) \propto \left[\prod_{j=0}^m P(B_j|I) \right] P(D|B_0B_1 \dots B_mI). \quad (16.14)$$

We want the Markov chain to explore the amplitude parameter space, but we don't want it to excessively waist time. All the amplitudes in an orthogonal model are estimated to be $\pm\sqrt{\langle\sigma^2\rangle}$, where $\langle\sigma^2\rangle$ is the mean-square residual given the model. Consequently, if we center the prior probability for an amplitude on the expected amplitude, T_j Eq. (16.16) below, and make the standard deviation of the prior very wide, then the prior probability for the amplitudes will do little more than keep the Markov chain in the physically meaningful region of the parameter space. Here is the prior actually used for the amplitudes:

$$P(B_j|I) = (2\pi\delta^2)^{-\frac{1}{2}} \exp\left\{-\frac{(T_j - B_j)^2}{2\delta^2}\right\} \quad (16.15)$$

where the expected amplitude, T_j , is given by

$$T_j \equiv \sum_{i=1}^N d_i H_j(t_i) \quad (16.16)$$

where N is the total number of data values in the data set. The standard deviation of this prior, δ , is 10 times larger than the expected root mean-square residual:

$$\delta = 10\sqrt{\langle\sigma^2\rangle} \quad (16.17)$$

with

$$\sqrt{\langle\sigma^2\rangle} = \sqrt{\frac{d^2 - \bar{h}^2}{N}}. \quad (16.18)$$

The quantity, $d^2 - \bar{h}^2$, is the total-squared residual given the polynomial. So the square root is the root mean-square residual given the polynomial order. The sufficient statistic, \bar{h}^2 , is the total-squared projection of the data onto the polynomial and is defined as

$$\bar{h}^2 \equiv \sum_{k=0}^m T_k^2. \quad (16.19)$$

Having assigned the prior probabilities, we must now assign the direct probability. The direct probability, $P(D|B_0B_1 \dots B_mI)$, is a marginal probability and is computed from the joint probability for the data and the standard deviation of the noise

$$P(D|B_0B_1 \dots B_mI) = \int P(\sigma D|B_0B_1 \dots B_mI) d\sigma \quad (16.20)$$

which we factor as

$$P(D|B_0B_1 \dots B_m I) = \int P(\sigma|I)P(D|\sigma B_0B_1 \dots B_m I)d\sigma. \quad (16.21)$$

Assigning a Jeffreys' prior to $P(\sigma|I)$ and a Gaussian likelihood, one obtains

$$P(B_0B_1 \dots B_m|DI) \propto \left[\prod_{j=0}^m P(B_j|I) \right] \int \frac{1}{\sigma} (2\pi\sigma^2)^{-\frac{N}{2}} \exp \left\{ -\frac{Q}{2\sigma^2} \right\} d\sigma \quad (16.22)$$

where we have left the prior probabilities in their symbolic form. Evaluating the integral over σ and substituting the prior probability for the amplitudes, Eq. (16.15), into Eq. (16.22), one obtains:

$$P(B_0B_1 \dots B_m|DI) \propto \left[\prod_{j=0}^m \exp \left\{ -\frac{(T_j - B_j)^2}{2\delta^2} \right\} \right] \left[\frac{Q}{2} \right]^{-\frac{N}{2}} \quad (16.23)$$

where we dropped some constant terms that cancel when this probability is normalized. The function Q is defined as

$$\begin{aligned} Q &\equiv \sum_{i=1}^N \left(d_i - \sum_{j=0}^m B_j H_j(t_i) \right)^2 \\ &= N\bar{d}^2 - 2 \sum_{j=0}^m B_j T_j + \sum_{j=0}^m B_j^2. \end{aligned} \quad (16.24)$$

One interesting note about the quantity Q , it does not depend on the individual data values, rather it depends on the total squared data value, the $N\bar{d}^2$, and it depends on the projection of the data onto the orthogonal functions, the T_j . Both of these items can be computed at the beginning of the calculation and used throughout with no further reference to the data. Consequently, the Given Polynomial Order runs very quickly. Also, note that the function Q could have been written as a single summation rather than two. If the standard deviation for the noise is known, the posterior probability for the B_j can be factored into a product of probabilities for each amplitude separately, i.e., the amplitudes of the orthogonal polynomials may be estimated separately, they don't have to be estimated jointly. Finally, because each amplitude can be estimated separately, one can simply plot the posterior probability for each amplitude, there is no need to use a Markov chain Monte Carlo simulation to sample the joint posterior. However, joint estimation is required after marginalizing out the standard deviation for the noise. The joint estimation is done using a Markov chain Monte Carlo simulation to sample the joint posterior probability for the amplitudes, Eq. (16.23).

16.2 Outputs From the Given Polynomial Order Package

The Text outputs files from the Given Polynomial Order package consist of: "Bayes.prob.model," "BayesPolGiven.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

Figure 16.2: Given Polynomial Order Scatter Plot

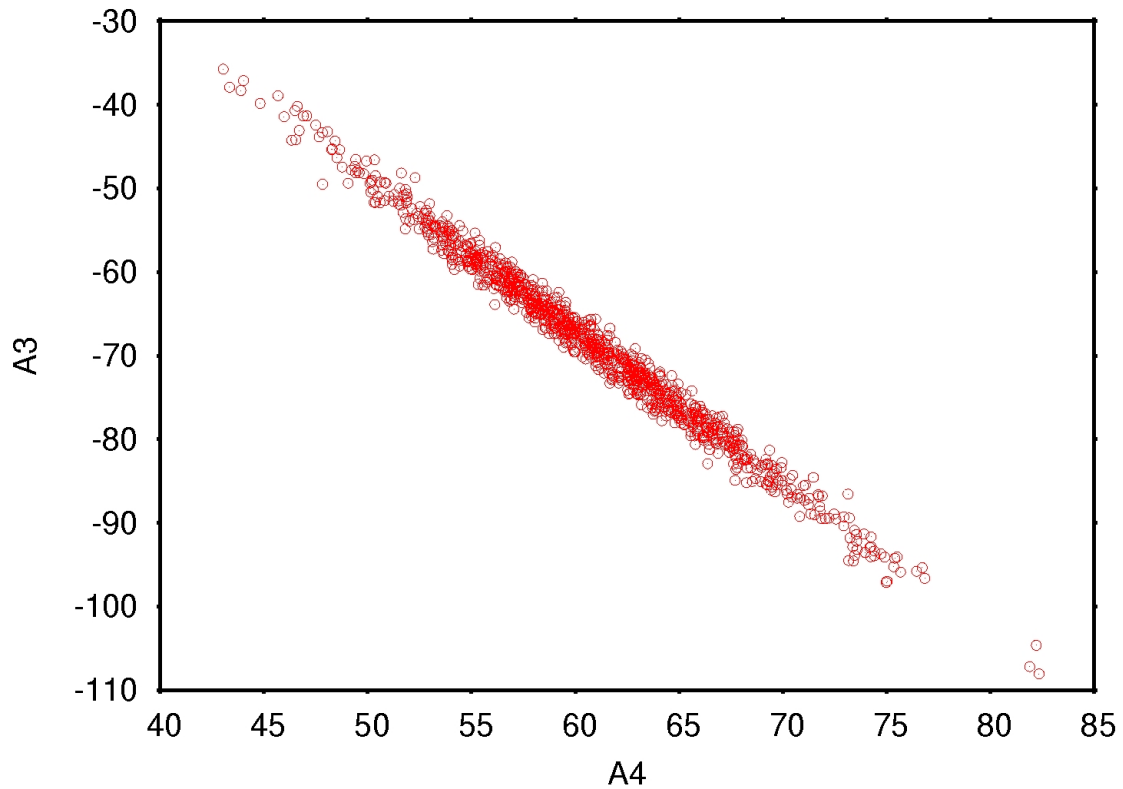


Figure 16.2 The expansion coefficients in a nonorthogonal polynomial expansion tend to be highly correlated. Plotted here is a scatter plot of the 3rd and 4th order expansion coefficients, A_3 and A_4 , as generated by a 6th order expansion of the 6th order polynomial test data. This test data can be downloaded using the “Files” menu.

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 each A_j in the given model. And because estimation of the amplitudes in polynomial models tend to be highly correlated, there are covariance plots to help illustrate these correlations. These covariance plots are scatter plots. The scatter plots are generated from the samples drawn from the Markov chain Monte Carlo simulation. In a typical run, there might be 50 simulations and 30 repeats giving a total of 1500 simulations. Each of these simulations contain the estimated parameters from one Markov chain Monte Carlo simulation. A typical scatter plot just put a dot in the plot at the location of parameter 1 versus parameter 2. In this package that would correspond to plotting A_j versus A_k . In Fig. 16.2, A_3 versus A_4 is plotted. The data used to generate this figure are the 6th order polynomial expansion data available in our test data kit. This test data can be downloaded using the “Files” menu. The covariance plot shown in Fig. 16.2 is the one generated

form the A_3 and A_4 expansion coefficients in a 6th order expansion of this data. For these two parameters there is a strong correlation, when A_3 increases the A_4 parameter decreases to counter the effect of changing A_3 . Uncorrelated parameters, by contrast, will have elliptical scatter plots with the major and minor axis aligned with coordinate system. The number of possible scatter plots is $m(m+1)$ where m is the order of the polynomial. Because the number of scatter plots can become large very quickly, the package only outputs a representative sample of these plots.

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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](#)
 - Procpair, [178](#)
 - Real Constant, [184](#)
 - Relative Amplitude, [183](#)
 - Resonance Model, [185](#)
 - Shim Order, [182](#)
 - Spectrometer Frequency, [182](#)
 - Text Parameters, [178](#)
 - Total Complex Data Values, [181](#)
 - Total Data Values, [181](#)
 - Total Sampling Time, [182](#)
 - True Reference, [182](#)

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

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

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