

Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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Contents

Manual Status	16
1 An Overview Of The Bayesian Analysis Software	19
1.1 The Server Software	19
1.2 The Client Interface	22
1.2.1 The Global Pull Down Menus	24
1.2.2 The Package Interface	24
1.2.3 The Viewers	27
2 Installing the Software	29
3 the Client Interface	33
3.1 The Global Pull Down Menus	35
3.1.1 the Files menu	35
3.1.2 the Packages menu	40
3.1.3 the WorkDir menu	45
3.1.4 the Settings menu	46
3.1.5 the Utilities menu	50
3.1.6 the Help menu	50
3.2 The Submit Job To Server area	51
3.3 The Server area	52
3.4 Interface Viewers	52
3.4.1 the Ascii Data Viewer	53
3.4.2 the fid Data Viewer	53
3.4.3 Image Viewer	59
3.4.3.1 the Image List area	59
3.4.3.2 the Set Image area	62
3.4.3.3 the Image Viewing area	62
3.4.3.4 the Grayscale area on the bottom	63
3.4.3.5 the Pixel Info area	63
3.4.3.6 the Image Statistics area	64
3.4.4 Prior Viewer	65
3.4.5 Fid Model Viewer	68
3.4.5.1 The fid Model Format	70

3.4.5.2	The Fid Model Reports	71
3.4.6	Plot Results Viewer	71
3.4.7	Text Results Viewer	74
3.4.8	Files Viewer	80
3.5	Common Interface Plots	80
3.5.1	Data, Model And Residual Plot	81
3.5.2	Posterior Probability For A Parameter	82
3.5.3	Maximum Entropy Histograms	83
3.5.4	Markov Monte Carlo Samples	83
3.5.5	Probability Vs Parameter Samples plot	86
3.5.6	Expected Log Likelihood Plot	88
3.5.7	Scatter Plots	88
3.5.8	Logarithm of the Posterior Probability Plot	91
3.5.9	Fortran/C Code Viewer	91
3.5.9.1	Fortran/C Model Viewer Popup Editor	94
4	An Introduction to Bayesian Probability Theory	99
4.1	The Rules of Probability Theory	99
4.2	Assigning Probabilities	102
4.3	Example: Parameter Estimation	109
4.3.1	Define The Problem	110
4.3.1.1	The Discrete Fourier Transform	110
4.3.1.2	Aliases	113
4.3.2	State The Model—Single-Frequency Estimation	114
4.3.3	Apply Probability Theory	115
4.3.4	Assign The Probabilities	118
4.3.5	Evaluate The Sums and Integrals	120
4.3.6	How Probability Generalizes The Discrete Fourier Transform	123
4.3.7	Aliasing	126
4.3.8	Parameter Estimates	132
4.4	Summary and Conclusions	136
5	Given Exponential Model	137
5.1	The Bayesian Calculation	139
5.2	Outputs From The Given Exponential Package	141
6	Unknown Number of Exponentials	143
6.1	The Bayesian Calculations	145
6.2	Outputs From The Unknown Number of Exponentials Package	148
7	Inversion Recovery	151
7.1	The Bayesian Calculation	153
7.2	Outputs From The Inversion Recovery Package	154

8	Bayes Analyze	155
8.1	Bayes Model	159
8.2	The Bayes Analyze Model Equation	161
8.3	The Bayesian Calculations	167
8.4	Levenberg-Marquardt And Newton-Raphson	171
8.5	Outputs From The Bayes Analyze Package	176
8.5.1	The “bayes.params.nnnn” Files	177
8.5.1.1	The Bayes Analyze File Header	178
8.5.1.2	The Global Parameters	182
8.5.1.3	The Model Components	184
8.5.2	The “bayes.model.nnnn” Files	185
8.5.3	The “bayes.output.nnnn” File	186
8.5.4	The “bayes.probabilities.nnnn” File	190
8.5.5	The “bayes.log.nnnn” File	193
8.5.6	The “bayes.status.nnnn” and “bayes.accepted.nnnn” Files	196
8.5.7	The “bayes.model.nnnn” File	197
8.5.8	The “bayes.summary1.nnnn” File	198
8.5.9	The “bayes.summary2.nnnn” File	199
8.5.10	The “bayes.summary3.nnnn” File	200
8.6	Bayes Analyze Error Messages	200
9	Big Peak/Little Peak	207
9.1	The Bayesian Calculation	209
9.2	Outputs From The Big Peak/Little Peak Package	216
10	Metabolic Analysis	219
10.1	The Metabolic Model	223
10.2	The Bayesian Calculation	225
10.3	The Metabolite Models	228
10.3.1	The IPGD_D2O Metabolite	228
10.3.2	The Glutamate.2.0 Metabolite	232
10.3.3	The Glutamate.3.0 Metabolite	235
10.4	The Example Metabolite	236
10.5	Outputs From The Bayes Metabolite Package	238
11	Find Resonances	239
11.1	The Bayesian Calculations	241
11.2	Outputs From The Bayes Find Resonances Package	246
12	Diffusion Tensor Analysis	247
12.1	The Bayesian Calculation	249
12.2	Using The Package	254
13	Big Magnetization Transfer	259
13.1	The Bayesian Calculation	259
13.2	Outputs From The Big Magnetization Transfer Package	262

14 Magnetization Transfer	265
14.1 The Bayesian Calculation	267
14.2 Using The Package	271
15 Magnetization Transfer Kinetics	275
15.1 The Bayesian Calculation	277
15.2 Using The Package	281
16 Given Polynomial Order	285
16.1 The Bayesian Calculation	287
16.1.1 Gram-Schmidt	287
16.1.2 The Bayesian Calculation	288
16.2 Outputs From the Given Polynomial Order Package	290
17 Unknown Polynomial Order	293
17.1 Bayesian Calculations	295
17.1.1 Assigning Priors	296
17.1.2 Assigning The Joint Posterior Probability	297
17.2 Outputs From the Unknown Polynomial Order Package	299
18 Errors In Variables	303
18.1 The Bayesian Calculation	305
18.2 Outputs From The Errors In Variables Package	308
19 Behrens-Fisher	311
19.1 Bayesian Calculation	311
19.1.1 The Four Model Selection Probabilities	314
19.1.1.1 The Means And Variances Are The Same	315
19.1.1.2 The Mean Are The Same And The Variances Differ	317
19.1.1.3 The Means Differ And The Variances Are The Same	318
19.1.1.4 The Means And Variances Differ	319
19.1.2 The Derived Probabilities	320
19.1.3 Parameter Estimation	321
19.2 Outputs From Behrens-Fisher Package	322
20 Enter Ascii Model	329
20.1 The Bayesian Calculation	331
20.1.1 The Bayesian Calculations Using Eq. (20.1)	331
20.1.2 The Bayesian Calculations Using Eq. (20.2)	332
20.2 Outputs Form The Enter Ascii Model Package	335
22 Enter Ascii Model Selection	341
22.1 The Bayesian Calculations	343
22.1.1 The Direct Probability With No Amplitude Marginalization	344
22.1.2 The Direct Probability With Amplitude Marginalization	346
22.1.2.1 Marginalizing the Amplitudes	347
22.1.2.2 Marginalizing The Noise Standard Deviation	352

22.2	Outputs Form The Enter Ascii Model Package	353
26	Phasing An Image	395
26.1	The Bayesian Calculation	396
26.2	Using The Package	402
27	Phasing An Image Using Non-Linear Phases	405
27.1	The Model Equation	405
27.2	The Bayesian Calculations	407
27.3	The Interfaces To The Nonlinear Phasing Routine	409
28	Analyze Image Pixel	411
28.1	Modification History	413
29	The Image Model Selection Package	415
29.1	The Bayesian Calculations	417
29.2	Outputs Form The Image Model Selection Package	418
A	Ascii Data File Formats	423
A.1	Ascii Input Data Files	423
A.2	Ascii Image File Formats	424
A.3	The Abscissa File Format	425
B	Markov chain Monte Carlo With Simulated Annealing	439
B.1	Metropolis-Hastings Algorithm	440
B.2	Multiple Simulations	441
B.3	Simulated Annealing	442
B.4	The Annealing Schedule	442
B.5	Killing Simulations	443
B.6	the Proposal	444
C	Thermodynamic Integration	445
D	McMC Values Report	449
E	Writing Fortran/C Models	455
E.1	Model Subroutines, No Marginalization	455
E.2	The Parameter File	458
E.3	The Subroutine Interface	460
E.4	The Subroutine Declarations	462
E.5	The Subroutine Body	463
E.6	Model Subroutines With Marginalization	464
F	the Bayes Directory Organization	469
G	4dfp Overview	471

H Outlier Detection

Bibliography

List of Figures

1.1	The Start Up Window	23
1.2	Example Package Exponential Interface	25
2.1	Installation Kit For The Bayesian Analysis Software	31
3.1	The Start Up Window	34
3.2	The Files Menu	35
3.3	The Files/Load Image Submenu	37
3.4	The Packages Menu	41
3.5	The Working Directory Menu	46
3.6	The Working Directory Information Popup	47
3.7	The Settings Pull Down Menu	47
3.8	The McMC Parameters Popup	48
3.9	The Edit Server Popup	49
3.10	The Submit Job Widgets	51
3.11	The Server Widgets Group	52
3.12	The Ascii Data Viewer	54
3.13	The Fid Data Viewer	55
3.14	Fid Data Display Type	56
3.15	Fid Data Options Menu	58
3.16	The Image Viewer	60
3.17	The Image Viewer Right Mouse Popup Menu	61
3.18	The Prior Probability Viewer	66
3.19	The Fid Model Viewer	69
3.20	The Plot Results Viewer	72
3.21	Plot Information Popup	73
3.22	The Text Results Viewer	75
3.23	The Bayes Condensed File	78
3.24	Data, Model, And Resid Plot	81
3.25	The Parameter Posterior Probabilities	82
3.26	The Maximum Entropy Histograms	84
3.27	The Parameter Samples Plot	85
3.28	Posterior Probability Vs Parameter Value	86
3.29	Posterior Probability Vs Parameter Value, A Skewed Example	87
3.30	The Expected Value Of The Logarithm Of The Likelihood	89

3.31	The Scatter Plots	90
3.32	The Logarithm Of The Posterior Probability By Repeat Plot	92
3.33	The Fortran/C Model Viewer	93
3.34	The Fortran/C Code Editor	95
4.1	Frequency Estimation Using The DFT	112
4.2	Aliases	113
4.3	Nonuniformly Nonsimultaneously Sampled Sinusoid	127
4.4	Alias Spacing	128
4.5	Which Is The Critical Time	130
4.6	Example, Frequency Estimation	131
4.7	Estimating The Sinusoids Parameters	133
5.1	The Given And Unknown Number Of Exponential Package Interface	138
6.1	The Unknown Exponential Interface	144
6.2	The Distribution Of Models	149
6.3	The Posterior Probability For Exponential Model	150
7.1	The Inversion Recovery Interface	152
8.1	Bayes Analyze Interface	156
8.2	Bayes Analyze Fid Model Viewer	160
8.3	The Bayes Analyze File Header	179
8.4	The bayes.noise File	180
8.5	Bayes Analyze Global Parameters	183
8.6	The Third Section Of The Parameter File	184
8.7	Example Of An Initial Model In The Output File	187
8.8	Base 10 Logarithm Of The Odds	187
8.9	A Small Sample Of The Output Report	188
8.10	Bayes Analyze Uncorrelated Output	189
8.11	The bayes.proBABILITIES.nnnn File	191
8.12	The bayes.log.nnnn File	193
8.13	The bayes.status.nnnn File	196
8.14	The bayes.model.nnnn File	197
8.15	The bayes.model.nnnn File Uncorrelated Resonances	198
8.16	Bayes Analyze Summary Header	198
8.17	The Summary2 (Best Summary)	199
8.18	The Summary3 Report	201
9.1	The Big Peak/Little Peak Interface	208
9.2	The Time Dependent Parameters	218
10.1	The Bayes Metabolite Interface	220
10.2	The Bayes Metabolite Viewer	222
10.3	Bayes Metabolite Parameters And Probabilities List	227
10.4	The IPGD_D20 Metabolite	229

10.5	Bayes Metabolite IPGD_D20 Spectrum	230
10.6	Bayes Metabolite, The Fraction of Glucose	231
10.7	Glutamate Example Spectrum	233
10.8	Estimating The F_{c0} , y and F_{a0} Parameters	236
10.9	Bayes Metabolite, The Ethyl Ether Example	237
11.1	The Find Resonances Interface With The Ethyl Ether Spectrum	240
12.1	The Diffusion Tensor Package Interface	248
12.2	Diffusion Tensor Parameter Estimates	256
12.3	Diffusion Tensor Posterior Probability For The Model	257
13.1	The Big Magnetization Package Interface	260
13.2	Big Magnetization Transfer Example Fid	263
13.3	Big Magnetization Transfer Expansion	263
13.4	Big Magnetization Transfer Peak Pick	264
14.1	The Magnetization Transfer Package Interface	266
14.2	Magnetization Transfer Package Peak Picking	272
14.3	Magnetization Transfer Example Data	273
14.4	Magnetization Transfer Example Spectrum	274
15.1	Magnetization Transfer Kinetics Package Interface	276
15.2	Magnetization Transfer Kinetics Package Arrhenius Plot	282
15.3	Magnetization Transfer Kinetics Water Viscosity Table	283
16.1	Given Polynomial Order Package Interface	286
16.2	Given Polynomial Order Scatter Plot	291
17.1	Unknown Polynomial Order Package Interface	294
17.2	The Distribution of Models On The Console Log	298
17.3	The Posterior Probability For The Polynomial Order	300
18.1	The Errors In Variables Package Interface	304
18.2	The McMC Values File Produced By The Errors In Variables Package	310
19.1	The Behrens-Fisher Interface	312
19.2	Behrens-Fisher Hypotheses Tested	313
19.3	Behrens-Fisher Console Log	323
19.4	Behrens-Fisher Status Listing	324
19.5	Behrens-Fisher McMC Values File, The Preamble	325
19.6	Behrens-Fisher McMC Values File, The Middle	326
19.7	Behrens-Fisher McMC Values File, The End	327
20.1	Enter Ascii Model Package Interface	330
22.1	The Enter Ascii Model Selection Package Interface	342

26.1	Absorption Model Images	396
26.2	The Interface To The Image Phasing Package	397
26.3	Linear Phasing Package The Console Log	403
27.1	Nonlinear Phasing Example	406
27.2	The Interface To The Nonlinear Phasing Package	410
28.1	The Interface To The Analyze Image Pixels Package	412
29.1	The Interface To The Image Model Selection Package	416
29.2	Single Exponential Example Image	419
29.3	Single Exponential Example Data	420
29.4	Posterior Probability For The ExpOneNoConst Model	421
A.1	Ascii Data File Format	424
D.1	The McMC Values Report Header	450
D.2	McMC Values Report, The Middle	451
D.3	The McMC Values Report, The End	452
E.1	Writing Models A Fortran Example	456
E.2	Writing Models A C Example	457
E.3	Writing Models, The Parameter File	459
E.4	Writing Models Fortran Declarations	463
E.5	Writing Models Fortran Example	466
E.6	Writing Models The Parameter File	467
G.1	Example FDF File Header	473
H.1	The Posterior Probability For The Number of Outliers	476
H.2	The Data, Model and Residual Plot With Outliers	478

List of Tables

8.1	Multiplet Relative Amplitudes	165
8.2	Bayes Analyze Models	181
8.3	Bayes Analyze Short Descriptions	195

Chapter 20

Enter Ascii Model

The Enter Ascii Model Package allows you to enter a model of your own and then use Bayesian probability theory to analyze that model.¹ To use this package you do not have to have either Fortran or C installed on your server. However, If you do not have either Fortran or C installed, the only models you will be able to use are the system models. Consequently, installing both Fortran and C is strongly recommended. The interface to this package is shown in Fig. 20.1 To use this package, you must do the following:

Select the “Enter Ascii Model” package from the Package menu.

Load a Fortran or C model using the “System” or “User” buttons in the “Load And Build Model” widget group.

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. The format of the Ascii data that must be loaded is dependent on the model. Usually the data are two column Ascii, however, in general this package takes multicolumn Ascii data with a multicolumn abscissa. See Appendix A for a detailed description of the Ascii data files used by the Bayesian Analysis software.

Build the model using the “Build” button.

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

Review the prior probabilities for the loaded model 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.

¹I would like to build a system library of predefined models. If you have models that you think would be of general use, I would like to hear from you. To have one of your models included, I would need the source code, the parameter file, a brief description of the model equations and data requirements.

Figure 20.1: Enter Ascii Model Package Interface

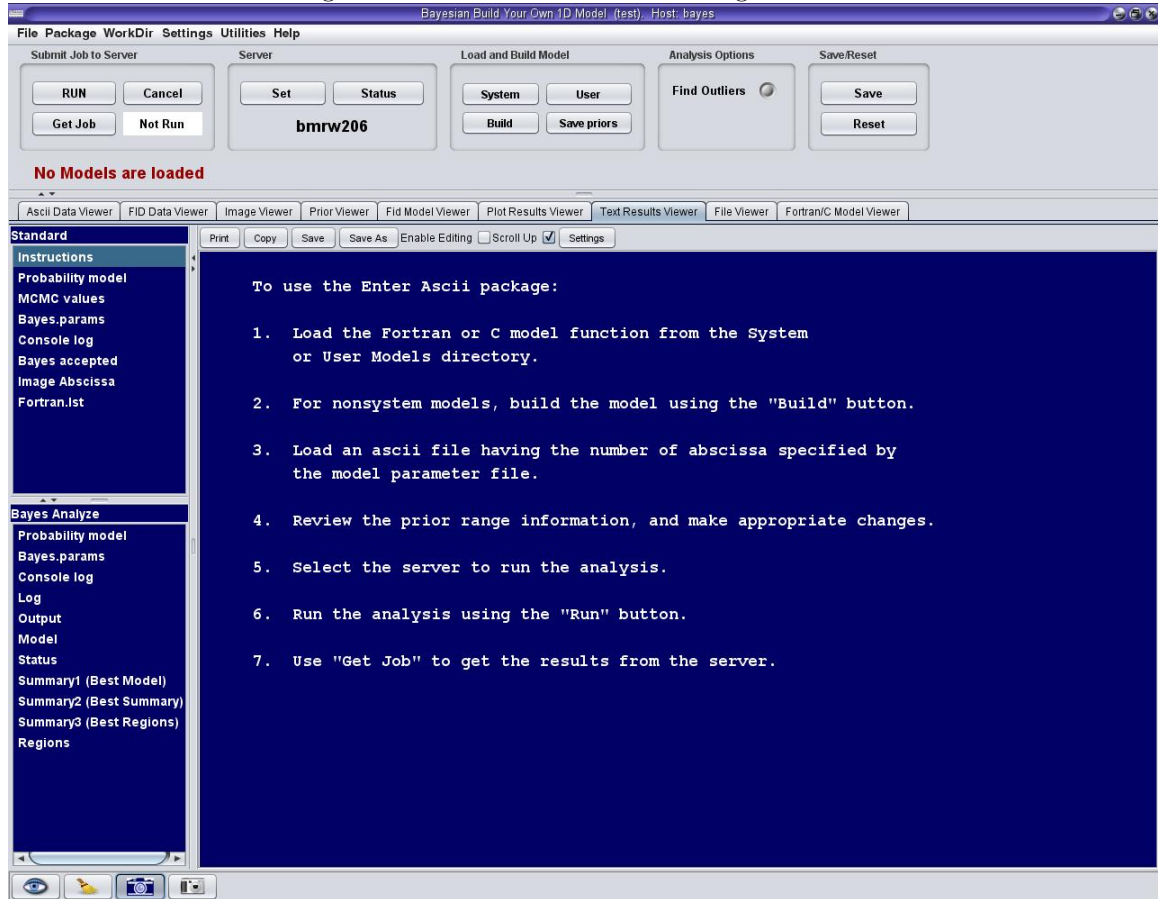


Figure 20.1: All packages that allow the user to load a Fortran or C model have the buttons titled “Load and Build Model.” These buttons allow you to load a model from either the system directory or from you user directory. They allow you to compile a model and save the current prior settings. Additionally, using the “Fortran/C Model Viewer” you can edit, modify and create models, see Appendix E for more on creating Fortran and C models.

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.

20.1 The Bayesian Calculation

The calculation done by Enter Ascii Model Package is a parameter estimation calculation. However, there are two distinct functional forms for the model that are used: one using marginalization over the amplitudes, and one that does not. The model function that does not use marginalization is given by:

$$d_j(t_i) = U_j(t_i, r_1, r_2, \dots) + n_j(t_i) \tag{20.1}$$

where $d_j(t_i)$ represents a data item in the j th data set at abscissa value t_i and t_i may be vector valued. $U_j(t_i, r_1, r_2, \dots)$ is the model function. r_j are the various parameters appearing in the model including any amplitudes that may be present, and $n_j(t_i)$ represents noise in the j th data set at abscissa t_i . Because, this model does not marginalize out the amplitudes, it is possible to restrict the amplitudes ranges using the prior probabilities.

The other model used by this package assumes the amplitudes are to be marginalized from the joint posterior probability for the parameters. The model equation that uses marginalization is similar

$$d_j(t_i) = \sum_{\ell=1}^m A_{jk} G_{j\ell}(t_i, r_1, r_2, \dots) + n_j(t_i) \tag{20.2}$$

where the amplitudes are labeled A_{jk} meaning the k th amplitude in the j th data set, the sum is over all of the amplitudes in the model, $G_{j\ell}(t_i, r_1, r_2, \dots)$ is the ℓ th model function in the j th data set evaluated at abscissa t_i and this model equation implicitly assumes that each data set contains same number of amplitudes.

20.1.1 The Bayesian Calculations Using Eq. (20.1)

To compute the marginal posterior probability for each parameter using Eq. (20.1), a Markov chain Monte Carlo simulation is run targeting the joint posterior probability for all of the parameters. This joint posterior probability is represented symbolically by $P(r_1 r_2 \dots | DI)$. The joint posterior probability for the parameters is factored using Bayes' theorem to obtain

$$P(r_1 r_2 \dots | DI) \propto P(r_1 r_2 \dots | I) P(D | r_1 r_2 \dots I) \tag{20.3}$$

where D stands for all of the data in all of the data sets, $P(r_1 r_2 \dots \sigma_1 \dots | I)$, is factored into independent prior probabilities for each parameter:

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] P(D | r_1 r_2 \dots I) \tag{20.4}$$

where m is the total number of parameters in the model, The priors, $P(r_j | I)$, are specified in the input parameter file that describes the model. These prior are either the defaults, if you loaded the model from the system directory, or they are the priors set using the interface. Because we don't

know the functional form of these priors, we are going to leave them in symbolic form. Factoring the direct probability for the data into an independent direct probability for each data set, one obtains

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n P(D_j | r_1 r_2 \dots I) \quad (20.5)$$

as the joint posterior probability for the parameters. The direct probability for the data is a marginal likelihood, because the standard deviation of the noise prior probability is not present. Introducing a standard deviation of the noise prior probability, σ_j , for each data set, and using the rules of probability theory to remove these parameters, one obtains:

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n \left[\int P(\sigma_j | I) P(D_j | \sigma_j r_1 r_2 \dots I) d\sigma_j \right]. \quad (20.6)$$

We have reached the point in this calculation where one has no other choice than to assign probabilities to represent each of these probabilities and then to perform the indicated integrals. Assign a Jeffreys' prior to the prior probability for the noise standard deviation:

$$P(\sigma_j | I) \propto \frac{1}{\sigma_j}, \quad (20.7)$$

and assigning the direct probability for the data using a Gaussian of standard deviation σ_j one obtains

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n \left[\int \sigma_j^{-(N_j+1)} \exp \left\{ -\frac{Q_j(t_i, r_1, r_2, \dots)}{2\sigma_j^2} \right\} d\sigma_j \right]. \quad (20.8)$$

as the joint posterior probability for the parameters, where $Q_j(t_i, r_1, r_2, \dots)$ is given by:

$$Q_j(t_i, r_1, r_2, \dots) \equiv \sum_{i=1}^{N_j} [d_j(t_i) - U_j(t_i, r_1, r_2, \dots)]^2, \quad (20.9)$$

and is the total squared residual and is essentially χ^2 . Evaluating the integral over the standard deviation of the noise, one obtains

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n \left[\frac{Q_j(t_i, r_1, r_2, \dots)}{2} \right]^{-\frac{N_j}{2}} \quad (20.10)$$

as the joint posterior probability for the parameters, where we have dropped a number of constants that make no difference in this parameter estimation problem.

20.1.2 The Bayesian Calculations Using Eq. (20.2)

To compute the marginal posterior probability for each parameter using Eq. (20.2), a Markov chain Monte Carlo simulation is run targeting the joint posterior probability for all of the nonlinear parameters. In this context, nonlinear means all of the parameters appearing in the model in a

nonlinear fashion, i.e., all of the parameters except the amplitudes. This joint posterior probability is represented symbolically by $P(r_1 r_2 \dots | DI)$. The joint posterior probability for the nonlinear parameters is factored using Bayes' theorem to obtain

$$P(r_1 r_2 \dots | DI) \propto P(r_1 r_2 \dots | I) P(D | r_1 r_2 \dots I) \quad (20.11)$$

where D stands for all of the data in all of the data sets, the prior probability for all of the nonlinear parameters is represented by, $P(r_1 r_2 \dots \sigma_1 \dots | I)$, and we will factor it into independent prior probabilities for each parameter. Consequently, the joint posterior probability for all of the nonlinear parameters is given by

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{j=1}^m P(r_j | I) \right] P(D | r_1 r_2 \dots I) \quad (20.12)$$

where m is the total number of nonlinear parameters in the model, The priors, $P(r_j | I)$, are specified in the input parameter file that describes the model. These prior are either the defaults, if you loaded the model from the system directory, or they are the priors set using the interface. Because we don't know the functional form of these priors, we are going to leave them in symbolic form. Factoring the direct probability for the data into an independent direct probability for each data set, one obtains

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n P(D_j | r_1 r_2 \dots I) \quad (20.13)$$

as the joint posterior probability for the nonlinear parameters.

The direct probability for the data is a marginal likelihood, because neither the standard deviation of the noise prior probability nor the amplitudes are present. To proceed with this calculation, these parameters must be reintroduced into the joint posterior probability for the nonlinear parameters. Representing the standard deviation of the noise prior probability for each data set as σ_j and $\{A\}_j$ as all of the amplitudes in the j th data set, one obtains

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n \int P(D_j \sigma_j \{A\}_j | r_1 r_2 \dots I) d\sigma_j d\{A\}_j \quad (20.14)$$

as the joint posterior probability for the parameters. Factoring the right-hand side of this equation, one obtains

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n \int P(\sigma_j | I) P(\{A\}_j | I) P(D_j | \sigma_j \{A\}_j r_1 r_2 \dots I) d\sigma_j d\{A\}_j \quad (20.15)$$

where $P(\sigma_j | I)$ is the prior probability for the standard deviation of the noise prior probability in the j th data set. Similarly, $P(\{A\}_j | I)$ is the joint prior probability for the amplitudes in the j th data set. If we assume the amplitudes are logically independent, then the joint prior probability for the amplitudes, $P(\{A\}_j | I)$, can be factored into a product of prior probabilities for each amplitude:

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n \int P(\sigma_j | I) \left[\prod_{k=1}^{\nu} P(A_{jk} | I) \right] P(D_j | \sigma_j \{A\}_j r_1 r_2 \dots I) d\sigma_j d\{A\}_j \quad (20.16)$$

where $P(A_{jk}|I)$ is the prior probability for the k th amplitude in the j th data set, and ν is the number of data sets. We will assign a zero-mean Gaussian prior probability for each amplitudes. This Gaussian prior probability is given by

$$P(A_{jk}|I) \propto \left(\frac{2\pi\sigma_j^2}{\gamma^2 g_{jkk}} \right)^{-\frac{1}{2}} \exp \left\{ -\frac{A_{jk}^2 \gamma^2 g_{jkk}}{2\sigma_j^2} \right\} \quad (20.17)$$

where

$$g_{jkl} \equiv \sum_{i=1}^{N_j} G_{jk}(t_i) G_{j\ell}(t_i) \quad (20.18)$$

and γ is used to control the width of this prior probability. The reason for this particular functional form is that it allows one to evaluate the integrals over the amplitudes in a concise functional form that aids in doing the numerical calculations. Substituting the prior probability for the amplitudes, Eq. (20.17), into the joint posterior probability for the parameters, Eq. 20.16,

$$\begin{aligned} P(r_1 r_2 \dots | DI) &\propto \left[\prod_{l=1}^m P(r_l | I) \right] \\ &\times \prod_{j=1}^n \left[\int \frac{1}{\sigma_j} \left(\frac{2\pi\sigma_j^2}{\gamma^2 g_{j11} \dots g_{j\nu\nu}} \right)^{-\frac{\nu}{2}} \right. \\ &\times \exp \left\{ -\sum_{k=1}^{\nu} \frac{A_{jk}^2 \gamma^2 g_{jkk}}{2\sigma_j^2} \right\} \\ &\times \left. P(D_j | \sigma_j \{A\}_j r_1 r_2 \dots I) d\sigma_j d\{A\}_j \right] \end{aligned} \quad (20.19)$$

and assigning a Gaussian for the direct probability for the data, $P(D_j | \sigma_j \{A\}_j r_1 r_2 \dots I)$, one obtains:

$$\begin{aligned} P(r_1 r_2 \dots | DI) &\propto \left[\prod_{l=1}^m P(r_l | I) \right] \\ &\times \prod_{j=1}^n \left[\int \frac{1}{\sigma_j} \left(\frac{2\pi\sigma_j^2}{\gamma^2 g_{j11} \dots g_{j\nu\nu}} \right)^{-\frac{\nu}{2}} \right. \\ &\times \exp \left\{ -\sum_{k=1}^{\nu} \frac{A_{jk}^2 \gamma^2 g_{jkk}}{2\sigma_j^2} \right\} \\ &\times \left. (2\pi\sigma_j^2)^{-\frac{N_j}{2}} \exp \left\{ -\sum_{i=1}^{N_j} \frac{(d_{ji} - \sum_{k=1}^{\nu} A_{jk} G_{jk}(t_i, r_1 \dots))^2}{2\sigma_j} \right\} d\sigma_j d\{A\}_j \right]. \end{aligned} \quad (20.20)$$

After evaluating the integrals over the amplitudes, one obtains

$$P(r_1 r_2 \dots | DI) \propto \left[\prod_{l=1}^m P(r_l | I) \right] \prod_{j=1}^n \left[\frac{\gamma^2}{g_{j11} \dots g_{j\nu\nu}} \right] |g_{jkl}|^{-\frac{1}{2}} \left[\frac{Q_j(r_1 r_2 \dots)}{2} \right]^{-\frac{N_j}{2}} \quad (20.21)$$

with

$$Q_j(r_1 r_2 \dots) \equiv \sum_{i=1}^{N_j} \left[d_{ji} - \sum_{\ell=1}^{\nu} \hat{A}_{j\ell} G_{j\ell}(t_i r_1 r_2 \dots) \right]^2, \quad (20.22)$$

$|g_{jkl}|$ is the magnitude of the determinate of the g_{jkl} matrix defined in Eq. (20.18) and the amplitudes $\hat{a}_{j\ell}$ are given by the solution to

$$\sum_{k=1}^{\nu} g_{jk\ell} \hat{A}_{j\ell} = T_{j\ell} \quad (20.23)$$

with the right-hand side of this equation given by:

$$T_{j\ell} = \sum_{i=1}^{N_j} d_j(t_i) G_{j\ell}(t_i). \quad (20.24)$$

See [2], and [11] for more on how the integrals over the amplitudes are evaluated. Equation 20.21 is the joint posterior probability for the nonlinear parameters that is targeted by the Markov chain Monte Carlo simulations. These simulations only vary the nonlinear parameters, the amplitudes simply do not appear in the posterior probability. However, the amplitudes are output from the simulation. The output amplitudes are given by Eq. (20.23). Because these amplitudes are estimated for each value of the nonlinear parameters, there is as many samples from the distributions of the amplitudes as there is for each of the nonlinear parameters. Consequently, the model that use marginalization do output density functions for the amplitudes.

20.2 Outputs Form The Enter Ascii Model Package

The Text outputs files from the Enter Ascii Model packages consist of: “Bayes.prob.model,” “BayesModelAscii.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 3. 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 parameter in the currently loaded Fortran/C model. These output probability density functions are named

`ModelFileName.ParamName`

where `ModelFileName` is the name of the currently loaded model. For example, if you have a model named `MyFunnyExp` model, and it has a decay rate named `FunnyRate` the output file containing the posterior probability for `FunnyRate` would be named:

`MyFunnyExp.FunnyRate.`

This naming convention also applies to derived parameters. So, if in addition to generating samples for `FunnyRate`, you also generated samples from a derived inverse decay rate, which was called `FunnyDecayTime` then there would also be an output file named

`MyFunnyExp.FunnyDecayTime`

containing the posterior probability for the decay time. For more on writing Ascii models in either Fortran or C, see Appendix [E](#).

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