Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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: larry@bayes.wustl.edu

July 13, 2018
Contents

Manual Status

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
8 Bayes Analyze

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
<table>
<thead>
<tr>
<th>14 Magnetization Transfer</th>
<th>265</th>
</tr>
</thead>
<tbody>
<tr>
<td>14.1 The Bayesian Calculation</td>
<td>267</td>
</tr>
<tr>
<td>14.2 Using The Package</td>
<td>271</td>
</tr>
<tr>
<td>15 Magnetization Transfer Kinetics</td>
<td>275</td>
</tr>
<tr>
<td>15.1 The Bayesian Calculation</td>
<td>277</td>
</tr>
<tr>
<td>15.2 Using The Package</td>
<td>281</td>
</tr>
<tr>
<td>16 Given Polynomial Order</td>
<td>285</td>
</tr>
<tr>
<td>16.1 The Bayesian Calculation</td>
<td>287</td>
</tr>
<tr>
<td>16.1.1 Gram-Schmidt</td>
<td>287</td>
</tr>
<tr>
<td>16.1.2 The Bayesian Calculation</td>
<td>288</td>
</tr>
<tr>
<td>16.2 Outputs From the Given Polynomial Order Package</td>
<td>290</td>
</tr>
<tr>
<td>17 Unknown Polynomial Order</td>
<td>293</td>
</tr>
<tr>
<td>17.1 Bayesian Calculations</td>
<td>295</td>
</tr>
<tr>
<td>17.1.1 Assigning Priors</td>
<td>296</td>
</tr>
<tr>
<td>17.1.2 Assigning The Joint Posterior Probability</td>
<td>297</td>
</tr>
<tr>
<td>17.2 Outputs From the Unknown Polynomial Order Package</td>
<td>299</td>
</tr>
<tr>
<td>18 Errors In Variables</td>
<td>303</td>
</tr>
<tr>
<td>18.1 The Bayesian Calculation</td>
<td>305</td>
</tr>
<tr>
<td>18.2 Outputs From The Errors In Variables Package</td>
<td>308</td>
</tr>
<tr>
<td>19 Behrens-Fisher</td>
<td>311</td>
</tr>
<tr>
<td>19.1 Bayesian Calculation</td>
<td>311</td>
</tr>
<tr>
<td>19.1.1 The Four Model Selection Probabilities</td>
<td>314</td>
</tr>
<tr>
<td>19.1.1.1 The Means And Variances Are The Same</td>
<td>315</td>
</tr>
<tr>
<td>19.1.1.2 The Mean Are The Same And The Variances Differ</td>
<td>317</td>
</tr>
<tr>
<td>19.1.1.3 The Means Differ And The Variances Are The Same</td>
<td>318</td>
</tr>
<tr>
<td>19.1.1.4 The Means And Variances Differ</td>
<td>319</td>
</tr>
<tr>
<td>19.1.2 The Derived Probabilities</td>
<td>320</td>
</tr>
<tr>
<td>19.1.3 Parameter Estimation</td>
<td>321</td>
</tr>
<tr>
<td>19.2 Outputs From Behrens-Fisher Package</td>
<td>322</td>
</tr>
<tr>
<td>20 Enter Ascii Model</td>
<td>329</td>
</tr>
<tr>
<td>20.1 The Bayesian Calculation</td>
<td>331</td>
</tr>
<tr>
<td>20.1.1 The Bayesian Calculations Using Eq. (20.1)</td>
<td>331</td>
</tr>
<tr>
<td>20.1.2 The Bayesian Calculations Using Eq. (20.2)</td>
<td>332</td>
</tr>
<tr>
<td>20.2 Outputs From The Enter Ascii Model Package</td>
<td>335</td>
</tr>
<tr>
<td>21 Enter Ascii Model Selection</td>
<td>337</td>
</tr>
<tr>
<td>21.1 The Bayesian Calculations</td>
<td>339</td>
</tr>
<tr>
<td>21.1.1 The Direct Probability With No Amplitude Marginalization</td>
<td>340</td>
</tr>
<tr>
<td>21.1.2 The Direct Probability With Amplitude Marginalization</td>
<td>342</td>
</tr>
<tr>
<td>21.1.2.1 Marginalizing the Amplitudes</td>
<td>343</td>
</tr>
<tr>
<td>21.1.2.2 Marginalizing The Noise Standard Deviation</td>
<td>348</td>
</tr>
</tbody>
</table>
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
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 $F_{e0}$, $y$ 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 Magnitization Transfer Package Interface ......................................... 266
14.2 Magnitization Transfer Package Peak Picking .......................................... 272
14.3 Magnitization Transfer Example Data ..................................................... 273
14.4 Magnitization Transfer Example Spectrum ............................................... 274

15.1 Magnitization Transfer Kinetics Package Interface .................................... 276
15.2 Magnitization Transfer Kinetics Package Arrhenius Plot ............................ 282
15.3 Magnitization 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

21.1 The Enter Ascii Model Selection Package Interface ................................... 338
List of Tables

8.1 Multiplet Relative Amplitudes ........................................ 165
8.2 Bayes Analyze Models ...................................................... 181
8.3 Bayes Analyze Short Descriptions ................................. 195
Chapter 21

Enter Ascii Model Selection

The Enter Ascii Model Selection Package allows you to load one or more Ascii model and then use Bayesian probability theory to compute the posterior probability for the loaded model, thus allowing you to determine which model best accounts for the data. To use this package you do not have to have Fortran or C installed on your server. However, if you do not have Fortran or C installed, you must use the system models. Consequently, installing both Fortran and C is strongly recommended. The interface to this package is shown in Fig. 21. To use this package, you must do the following:

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

Load one or more 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 abscissas. 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 would normally be the next step. However, in this package it is assumed that you have previously compiled and tested each Ascii model, so this package does not have a “Build” button.

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

Review the prior probabilities for the loaded model using the Prior Viewer would normally be the next step. However, because multiple models are loaded and thus multiple parameter sets are loaded, we require the user to test his models prior to running this package. So there is no review of the prior probabilities in this package. You can test your models using either the Enter Ascii Model Package or the Test Ascii Model package and you can review and update the prior information using those packages.

\[^1\] I 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 21.1: The Enter Ascii Model Selection Package Interface

To use the Ascii Model Selection Package:

1. Using the Enter Ascii package, load your data and set all of the prior ranges for all of the models to be tested before attempting to use this model selection package.

2. Load up to 10 Fortran or C model functions from your User model directory. Note these models must use the same number of abscissa and data columns.

3. Load an ascii file having the number of data columns and abscissa columns specified by the models.

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

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

21.1 The Bayesian Calculations

In the model selection calculation done by the Enter Ascii Model Selection package, it assumes one has a set of models, \( U_j \equiv \{U_1, \ldots, U_m\} \), and one wishes to compute the posterior probability for each of the \( U_j \) models. These models can be loaded from the System directory or they can be loaded from the user directory. They don’t need to have common parameters, but they do need to have common data requirements. Each of these models will have a set of parameters associated with it and these parameters will be designated as \( \Omega_j \). The subscript \( j \) indicating that these are the parameters associated with model \( U_j \). The equation that relates model \( U_j \) to the data is given by

\[
d_k(t_i) = U_j(t_i, \Omega_j) + n_k(t_i)
\]  

(21.1)

where \( d_k(t_i) \) represents a data item in the \( k \)th data set, sampled at abscissa value \( t_i \). The \( t_i \) may be vector valued or it may be a single column of numbers. However, it must have the same number of columns in all loaded models. The noise is represented symbolically by \( n_k(t_i) \) and is the noise value in the \( k \)th data set sampled at abscissa value \( t_i \).

The posterior probability for each model \( U_j \) is given by Bayes’ theorem:

\[
P(U_j|DI) = \frac{P(U_j|I)P(D|U_jI)}{P(D|I)}
\]  

(21.2)

where \( P(U_j|DI) \) is the posterior probability for model \( U_j \) given the data and the prior information, \( P(U_j|I) \) is the prior probability for model \( U_j \) given only the prior information, \( P(D|U_jI) \) is the marginal direct probability for all of the data given the model \( U_j \) and the prior information. This term was called a direct probability because it is a probability for the data and it is a marginal probability because none of the parameters from model \( U_j \) appear, so they have been marginalized out. \( P(D|I) \) is a normalization constant that ensures the probabilities sum to one:

\[
\sum_{j=1}^{m} P(U_i|DI) = 1,
\]  

(21.3)

so

\[
\sum_{j=1}^{m} \frac{P(U_j|I)P(D|U_jI)}{P(D|I)} = 1,
\]  

(21.4)

and

\[
\sum_{j=1}^{m} P(U_j|I)P(D|U_jI) = P(D|I)
\]  

(21.5)
Equation (21.2) cannot be computed in this form because the marginal direct probability, $P(D|U_j I)$, cannot be assigned. However, the prior probability for the models, $P(U_j | I)$ can be assigned and in this calculation it is assigned as a uniform prior:

$$P(U_j | I) = \frac{1}{m}. \quad (21.6)$$

The marginal direct probability for the data given the model, $P(D|U_j I)$, can be computed if we reintroduce the model parameters $\Omega_j$ and then use the sum rule of probability theory to marginalize out these parameters

$$P(D|U_j I) = \int P(D|\Omega_j U_j I) d\Omega_j. \quad (21.7)$$

The probability on the right-hand side of this equation is the joint prior probability for the data and the $\Omega_j$ parameters given the model $U_j$ and the prior information $I$. Applying the product rule to factor the right-hand side of this equation, one obtains

$$P(D|U_j I) = \int P(\Omega_j | I) P(D|\Omega_j U_j I) d\Omega_j \quad (21.8)$$

where $P(D|\Omega_j U_j I)$ is the direct probability for the data given the parameters and the model, this direct probability is also called a likelihood and $P(\Omega_j | I)$ is the joint prior probability for the $\Omega_j$ parameters.

In the Bayesian Analysis software that implements this calculation, there are two types of Ascii models: those that do not use marginalization to remove the amplitudes and those that do. The functional form of the Ascii model is very different between these two types of Fortran/C codes. Consequently, the calculation for the marginal direct probability for the data given the model, $P(D|U_j I)$, must be split into two separate calculations: one that uses amplitude marginalization and one that does not.

### 21.1.1 The Direct Probability With No Amplitude Marginalization

In this subsection it will be assumed that the input model is one that has not defined any amplitudes and consequently there is no amplitude marginalization in the posterior probability for the parameters. So in this calculation the $\Omega_j$ parameters are given by $\Omega_j \in \{\omega_{j1}, \ldots, \omega_{j\nu_j}\}$ where $\nu_j$ is the number of parameters. The individual Ascii model parameters are designated by $\omega_{jk}$ and these parameters may include amplitudes, but if it does, the program that implements the calculation has no knowledge of them. Assuming logical independence of the parameters, i.e., knowing the value of one parameter would not help us in making inferences about the other parameters, then the joint prior probability for the $\Omega_j$ parameters can be factored into an independents prior probability for each parameter,

$$P(\Omega_j | I) = \prod_{k=1}^{\nu_j} P(\omega_{jk} | \Omega_j I) \quad (21.9)$$

where $P(\omega_{jk} | \Omega_j I)$ is the prior probability for the $k$ parameter in the $j$th model. The model $\Omega_j$ was include in the prior information because what prior we assign to the parameters will definitely be dependent on the model.

The likelihood, $P(D|\Omega_j U_j I)$, is the likelihood function for all of the data $D$. However, the data $D$ is made up of multiple data sets, $D \equiv \{D_1, \ldots, D_n\}$, where $n$ is the input number of data sets,
and each data set consists of \( N_j \) data values, so \( D_j \equiv \{ d_j(t_1), \ldots, d_j(t_{N_j}) \} \), where \( d_j(t_i) \) is a data item in the \( j \)th data set sampled at abscissa value \( t_i \). The number of data values in a given data set, \( N_j \), need not be the same from one data set to another. Assuming logical independence of the various data sets, the joint direct probability for the data, \( P(D|\Omega_j U_j I) \), can be written as

\[
P(D|\Omega_j U_j I) = \prod_{k=1}^{n} P(D_k|\Omega_j U_j I).
\]  

(21.10)

Each of the probabilities, \( P(D_k|\Omega_j U_j I) \), is a direct probability or likelihood for the data in the \( k \)th data set given the model, the parameters, and the prior information. Such direct probabilities are usually assigned using a Gaussian prior probability for the noise, then the likelihood for a single data set becomes

\[
P(D_k|\sigma_k \Omega_j U_j I) = (2\pi \sigma_k^2)^{-\frac{N_k}{2}} \exp \left\{ -\frac{Q_{jk}^2}{2\sigma_k^2} \right\}
\]  

(21.11)

where the standard deviations have been added to \( P(D_k|\Omega_j U_j I) \) because the right-hand side of this equation cannot be computed unless the standard deviations are known. The total squared residual, \( Q_{jk}^2 \), is defined as:

\[
Q_{jk}^2 \equiv \sum_{i=1}^{N_k} [d_k(t_i) - U_j(t_i, \Omega_j)]^2
\]  

(21.12)

in the \( k \)th data set given the \( j \)th model and its parameters \( \Omega_j \). Substituting Eq. (21.11) into Eq. (21.10) one obtains

\[
P(D\sigma_1 \cdots \sigma_n U_j I) = \prod_{k=1}^{n} (2\pi \sigma_k^2)^{-\frac{N_k}{2}} \exp \left\{ -\frac{Q_{jk}^2}{2\sigma_k^2} \right\}
\]  

(21.13)

as the direct probability for all of the data, where we have modified the notation to indicate that all of the \( \sigma_j \) must be given. Finally, substituting Eq. (21.13), Eq. (21.9) and Eq. (21.6) into Eq. (21.2) one obtains

\[
P(U_j|\sigma_1 \cdots \sigma_n DI) \propto \int \frac{1}{m} \left[ \prod_{k=1}^{n} P(\omega_{jk}|I) \right] \left[ \prod_{k=1}^{n} (2\pi \sigma_k^2)^{-\frac{N_k}{2}} \exp \left\{ -\frac{Q_{jk}^2}{2\sigma_k^2} \right\} \right] \, d\Omega_j
\]  

(21.14)

as the marginal posterior probability for model \( U_j \). In the package that processes this analysis, the prior probabilities are specified by the user. And because the prior probability for the model was assigned as uniform, it will cancel when this probability density function is normalized. A Markov chain Monte Carlo simulation is used to numerically integrate this equation and thus obtain the posterior probability for the models.

Often the standard deviation of the noise prior probability are not known, so Eq. (21.14) cannot be used. When the standard deviation are not known, one can remove the standard deviations using the rules of probability theory:

\[
P(U_j|DI) = \int P(\sigma_1 \cdots \sigma_n U_j|DI) d\sigma_1 \cdots d\sigma_n d\Omega_j.
\]  

(21.15)
Factoring the right-hand side using the product rule of probability theory, one obtains

$$P(U_j | DI) = \int P(\sigma_1 \cdots \sigma_n | I) P(U_j | \sigma_1 \cdots \sigma_n DI) d\sigma_1 \cdots d\sigma_n d\Omega_j.$$  \hspace{1cm} (21.16)

Assuming logical independence, the joint prior probability for the standard deviations can be factored to obtain:

$$P(U_j | DI) = \left[ \prod_{k=1}^{n} P(\sigma_j | I) \right] P(U_j | \sigma_1 \cdots \sigma_n DI) d\sigma_1 \cdots d\sigma_n d\Omega_j.$$  \hspace{1cm} (21.17)

Substituting Eq. (21.14) into Eq. (21.17) one obtains

$$P(U_j | DI) \propto \frac{1}{m} \int \left[ \prod_{k=1}^{\nu_j} P(\omega_{jk} | I) \right] \left[ \prod_{k=1}^{n} (2\pi \sigma_k)^{-\frac{N_k + 1}{2}} \exp \left\{ -\frac{Q_{jk}^2}{2\sigma_k^2} \right\} \right] d\sigma_1 \cdots d\sigma_n d\Omega_j.$$  \hspace{1cm} (21.18)

as the posterior probability for model \(U_j\) given the data and the prior information. The integrals of the standard deviations of the noise prior probability are gamma function integrals. We address those integrals in the next section when we consider the same calculation but with marginalization over the amplitudes. Here we are just going to give the result of marginalizing over the \(\sigma_k\):

$$P(U_j | DI) \propto \frac{1}{m} \int \left[ \prod_{k=1}^{\nu_j} P(\omega_{jk} | I) \right] \left[ \prod_{k=1}^{n} \frac{1}{2} \Gamma \left( \frac{N_k}{2} \right) Q_{jk} \right] d\Omega_j.$$  \hspace{1cm} (21.19)

For the details of how this integration is performed see subsection 21.1.2.2. When the standard deviation for the noise prior probability is known Eq. (21.18) is used in the numerical simulation that implements this calculation. Knowledge of the standard deviation of the noise prior probability usually comes about in image processing applications because in those applications it is possible to directly sample the noise. However, more often than not, no information is available about the standard deviation of the noise prior probability, then the posterior probability for the model independent of the standard deviations of the noise prior probability, Eq. (21.19), is used. The functional form of this equation is that of a Student’s \(t\)-distribution. The Markov chain Monte Carlo simulation that is used to evaluate the remaining integrals targets either Eq. (21.18) or Eq. (21.19) using a Monte Carlo simulation to draw samples from this posterior probability and then uses Monte Carlo integration to evaluate the posterior probability for the models.

### 21.1.2 The Direct Probability With Amplitude Marginalization

The above calculation assumes the amplitudes are not analytically marginalized out. However, the Bayesian Analysis software uses two types of models. One that does not explicitly marginalize out the amplitudes and one that does. The functional form of these models that marginalize out the amplitudes is a special subset of the from assumed above. The models that do not marginalize out the amplitudes may contain amplitudes, but they are not identified as such in the parameter file associated with the Fortran/C model; rather the amplitudes are just lumped in with the other nonlinear parameters. However, when the amplitudes are marginalized out, the amplitudes are made explicit in the Fortran/C model parameter file and the functional form of the Fortran/C model is different. Consequently, the calculation for the marginal posterior probability for the model is a bit different for these models.
The signal model used in the calculation when the amplitudes are marginalized out, starts out similar to the calculation where no marginalization occurs. The data are related to the \( j \)th model \( U_j \) by

\[
d_k(t_i) = U_j(t_i, B_j, \Omega_j) + n_k(t_i) \tag{21.20}
\]

where \( d_k(t_i) \) represents a data item in the \( k \)th data set that was sampled at abscissa value \( t_i \), \( n_k(t_i) \) represents the noise in the \( k \)th data set sampled at abscissa value \( t_i \), \( B_j \) is the set of all amplitudes appearing in the \( j \)th model, and \( \Omega_j \) is the set of all nonamplitude parameters, \( \Omega_j \in \{ \omega_{j1}, \ldots, \omega_{j\nu_j} \} \) and \( \nu_j \) is the number of nonamplitude parameters in the \( j \)th data set. These parameters will be referred to as the nonlinear parameters because they almost always appear in the model in a nonlinear fashion. The model, \( U_j \in \{ U_1, \ldots, U_m \} \), is one from the set of models that are being analyzed. When the amplitudes are marginalized out, it is assumed that the \( U_j(t_i, B_j, \Omega_j) \) have the following functional form:

\[
U_j(t_i, B_j, \Omega_j) = u_j \sum_{\ell=1}^{u_j} B_{jk\ell} G_{j\ell}(t_i, \Omega_j) \tag{21.21}
\]

where \( B_{jk\ell} \) is the \( \ell \)th amplitude of the \( j \)th model in the \( k \)th data set, and \( G_{j\ell}(t_i, \Omega_j) \) is the \( \ell \)th subcomponent of the \( j \)th model. Note that the \( G_{j\ell}(t_i, \Omega_j) \) do not depend on the amplitudes in any way; and in this model the only dependence on the amplitudes is a linear dependence. To given an example of this, suppose we are estimating a sum of \( u_j \) sinusoids, the model \( U_j(t_i, B_j, \Omega_j) \) would be given by

\[
U_j(t_i, B_j, \Omega_j) = u_j \sum_{\ell=1}^{u_j} B_{jk\ell} \cos(2\pi\omega_{j\ell} t_i + \theta_{j\ell}) \tag{21.22}
\]

and each submodel component, the \( G_{j\ell}(t_i, \Omega_j) \) are given by

\[
G_{j\ell}(t_i, \Omega_j) = \cos(2\pi\omega_{j\ell} t + \theta_{j\ell}). \tag{21.23}
\]

In this sinusoidal model, the sinusoids depend on the data sets through the amplitude and phase while the frequencies are common to all data sets.

21.1.2.1 Marginalizing the Amplitudes

To compute the posterior probability for the model when the amplitudes are marginalized out, we note that that the calculation begins where the previous calculation ends with Eq. (21.14). Rewriting Eq. (21.14) so as to separate out the amplitudes integrals from the integrals over the nonlinear parameters, one obtains

\[
P(U_j|D) \propto \frac{1}{m} \int \left[ \prod_{\ell=1}^{u_j} P(\omega_{j\ell}|I) \right] \left[ \prod_{k=1}^{n} \left( \prod_{z=1}^{u} P(B_{jkz}|I) \right) \right] \left( 2\pi\sigma_k \right)^{-N_k} \exp \left\{ - \frac{Q_{jk}^2}{2\sigma_k^2} \right\} dB_j d\Omega_j \tag{21.24}
\]

where \( u_j \) is the number of amplitudes in the \( j \)th model. The prior probability for the \( \ell \)th nonlinear parameter in the \( j \)th model is designated by \( P(\omega_{j\ell}|I) \). Finally, \( P(B_{jkz}|I) \) is the prior probability for the \( z \)th amplitude in the \( j \)th model of the \( k \)th data set. Substituting the model, Eq. (21.21), into
the definition of $Q_{jk}^2$, Eq. (21.12), we can obtain

$$Q_{jk}^2 \equiv \sum_{i=1}^{N_k} [d_k(t_i) - U_k(t_i, B_j, \Omega_j)]^2$$

$$= \sum_{i=1}^{N_k} \left[ d_k(t_i) - \sum_{\ell=1}^{u_j} B_{jk\ell} G_{j\ell}(t_i, \Omega_j) \right]^2.$$  \hspace{1cm} (21.25)

Multiplying out the brackets one obtains

$$Q_{jk}^2 = d_k(t_i) \cdot d_k(t_i) - 2 \sum_{\ell=1}^{u_j} B_{jk\ell} d_k(t_i) \cdot G_{j\ell}(t_i) + \sum_{\ell=1}^{u_j} \sum_{v=1}^{u_j} B_{jk\ell} B_{jkv} G_{j\ell}(t_i) \cdot G_{jv}(t_i) \hspace{1cm} (21.26)$$

where we are using the “.” notation to mean sum over time, so

$$d_k(t_i) \cdot G_{j\ell} = \sum_{i=1}^{N_k} d_k(t_i) G_{j\ell}(t_i). \hspace{1cm} (21.27)$$

And to compress the notation still further, we define

$$d_k^2 = d_k(t_i) \cdot d_k(t_i), \hspace{1cm} (21.28)$$

$$T_{jk\ell} = d_k(t_i) \cdot G_{j\ell}(t_i) \hspace{1cm} (21.29)$$

and

$$g_{j\ell v} = G_{j\ell}(t_i) \cdot G_{jv}(t_i) \hspace{1cm} (21.30)$$

so Eq. (21.26) becomes

$$Q_{jk}^2 = d_k^2 - 2 \sum_{\ell=1}^{u_j} B_{jk\ell} T_{jk\ell} + \sum_{\ell=1}^{u_j} \sum_{v=1}^{u_j} B_{jk\ell} B_{jkv} g_{j\ell v}. \hspace{1cm} (21.31)$$

To evaluate the integrals in Eq. (21.24), we must assign a prior probability for the amplitudes. A zero-mean Gaussian prior probability will be assigned for each amplitude. This Gaussian prior probability is given by

$$P(B_{jku}|I) \propto \left( \frac{2\pi \sigma_j^2}{\gamma^2 g_{juu}} \right)^{-\frac{1}{2}} \exp \left\{ -\frac{B_{jku}^2 \gamma^2 g_{juu}}{2\sigma_j^2} \right\} \hspace{1cm} (21.32)$$

where $\gamma$ is used to control the width of this prior probability, $\sigma_j$ is the standard deviation of the noise prior probability in the $j$th data set, and $g_{jku}$ was defined in Eq. (21.30). The reason for this particular 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 Eq. (21.32) and Eq. (21.31) into the posterior probability for the model, Eq. (21.24), one obtains

\[
P(U_j|DI) = \frac{1}{m} \int \left[ \prod_{l=1}^{v_j} P(\omega_{jl}|I) \right] \times \prod_{k=1}^{n} \left[ \frac{1}{\sigma_k} \prod_{\beta=1}^{u_{jk}} \left( \frac{2\pi\sigma_k^2}{\gamma^2g_{j\beta\beta}} \right)^{-\frac{1}{2}} \exp \left\{ -\frac{B_{jk\beta}^2\gamma^2g_{j\beta\beta}}{2\sigma_k^2} \right\} \right] \times (2\pi\sigma_k^2)^{-\frac{N_k}{2}} \exp \left\{ -\frac{1}{2\sigma_k^2} \left[ d_k(t_i)^2 - 2\sum_{\ell=1}^{u_j} B_{jk\ell}T_{jk\ell} + \sum_{\ell=1}^{u_j} \sum_{v=1}^{u_j} B_{jk\ell}B_{jkv}g'_{j\ell v} \right] \right\} \times dB_{jk1} \cdots dB_{jku_j} d\sigma_k d\Omega_j
\]

as the posterior probability for model \( U_j \). Expanding the product over \( \beta \), and simplifying this equation somewhat, one obtains

\[
P(U_j|DI) \propto \int \left[ \prod_{l=1}^{v_j} P(\omega_{jl}|I) \right] \prod_{k=1}^{n} \left[ \frac{1}{\sigma_k} (2\pi\sigma_k^2)^{-\frac{N_k+u_j}{2}} \gamma^{u_j}g_{j11} \cdots g_{ju_ju_j} \right] \times \exp \left\{ -\frac{1}{2\sigma_k^2} \left[ d_k(t_i)^2 - 2\sum_{\ell=1}^{u_j} B_{jk\ell}T_{jk\ell} + \sum_{\ell=1}^{u_j} \sum_{v=1}^{u_j} B_{jk\ell}B_{jkv}g'_{j\ell v} \right] \right\} \times dB_{jk1} \cdots dB_{jku_j} d\sigma_1 \cdots d\sigma_n d\Omega_j
\]

where

\[
g'_{j\ell v} = g_{j\ell v} (1 + \delta_{\ell v}\gamma^2)
\]

and \( \delta_{\ell v} \) is the Kronecker delta function. The Kronecker delta function is zero if \( l \neq v \) and its one if \( l = v \). In order to evaluate the amplitude integrals a change of variables and functions will be made. The \( g'_{j\ell v} \) matrix is positive definite and of rank \( u_j \). Let \( e_{\ell v} \) represent the \( v \)th component of the \( \ell \)th normalized eigenvector of \( g'_{j\ell v} \), then

\[
\sum_{v=1}^{u_j} g'_{j\ell v} e_{\ell v} = \lambda_{\ell} e_{\ell \beta}
\]

where \( \lambda_{\ell} \) is the \( \ell \)th eigenvalue of \( g_{j\ell v} \). The functions \( H_{j\ell}(t_i) \), defined as

\[
H_{j\ell}(t_i) = \frac{1}{\sqrt{\lambda_{\ell}}} \sum_{v=1}^{u_j} e_{\ell v} G_{jv}(t_i),
\]

are orthonormal, i.e.,

\[
\sum_{i=1}^{N_i} H_{j\ell}(t_i) H_{jv}(t_i) = \delta_{\ell v}
\]

where \( \delta_{\ell v} \) is the Kronecker delta function and it is these \( H_j \) functions that will be used in the calculation. The model Eq. (21.21) can be rewritten in terms of these orthonormal functions as

\[
U_j(t_i, A_j, \Omega_j) = \sum_{\ell=1}^{u_j} A_{j\ell} H_{j\ell}(t_i)
\]
and it is these \( A_{jk\ell} \) that will be used in a change of variables. The amplitudes \( B_{jk\ell} \) are linearly related to the \( A_{jk\ell} \) by

\[
B_{jk\ell} = \sum_{\beta=1}^{u_j} \frac{A_{jk\beta}e_{\beta\ell}}{\sqrt{\lambda_\beta}} \quad \text{and} \quad A_{jk\ell} = \sqrt{\lambda_\ell} \sum_{\beta=1}^{u_j} B_{jk\beta}e_{\beta\ell}. \tag{21.40}
\]

The volume elements in the \( k \)th data set is given by

\[
dB_{jk1} \cdots dB_{jk\nu_j} = \left| \frac{e_{j\nu}}{\sqrt{\lambda_v}} \right| dA_{jk1} \cdots dA_{jk\nu_j} \tag{21.41}
\]

\[
= \lambda_1^{-\frac{1}{2}} \cdots \lambda_u^{-\frac{1}{2}} dA_{jk1} \cdots dA_{jk\nu_j},
\]

The Jacobin is a function of the \( \Omega_j \) parameters but it is a constant as long as we are not integrating over the \( \Omega_j \) parameters. At the end of the calculation the linear relations between the \( A \)'s and \( B \)'s can be used to calculate the expected values of the \( B \)'s from the expected value of the \( A \)'s,

\[
E(B_{jk\ell}|\Omega_j DI) = \langle B_{jk\ell} \rangle = \sum_{\beta=1}^{u_j} \frac{(A_{jk\beta})e_{\beta\ell}}{\sqrt{\lambda_\beta}} \tag{21.42}
\]

and the same is true of the second posterior moments:

\[
E(B_{jk\ell}B_{jk\ell}|\Omega_j DI) = \langle B_{jk\ell}B_{jk\ell} \rangle = \sum_{\beta=1}^{u_j} \sum_{v=1}^{u_j} \frac{e_{\beta\ell}e_{v\ell}(A_{jk\beta}A_{jk\nu})}{\sqrt{\lambda_\beta\lambda_v}} \tag{21.43}
\]

where \( E(B_{jk\ell}|\Omega_j DI) \) means the expected value of the \( \ell \)th amplitude \( B_{jk\ell} \) in the \( j \)th model of the \( k \)th data set given the nonlinear \( \Omega_j \) parameters, the data \( D \) and the prior information \( I \). Substituting, Eq. (21.40) into Eq. (21.34) and using the definition of the \( H_j \) functions, Eq. (21.37) one can rewrite the posterior probability for the model as:

\[
P(U_j|DI) \propto \int \prod_{l=1}^{v_jk} \mathcal{P}(\omega_{jk\ell}|I) \prod_{k=1}^n \left[ \frac{1}{\sigma_k} \left( 2\pi \sigma_k^2 \right)^{-\frac{N_k}{2}} \gamma^{-\frac{N_k}{2}} \sum_{u_j} g_{j1} \cdots g_{ju_j} u_j \lambda_1^{-\frac{1}{2}} \cdots \lambda_u^{-\frac{1}{2}} \right]
\]

\[
\times \exp \left\{ -\frac{1}{2\sigma_k^2} \left[ d_k^2 - 2\sum_{\ell=1}^{u_j} A_{jk\ell}h_{jk\ell} + \sum_{v=1}^{u_j} A_{jk\ell}^2 \right] \right\}
\]

\[
\times dA_{jk1} \cdots dA_{jk\nu_j} d\sigma_1 \cdots d\sigma_n d\Omega_j \tag{21.44}
\]

where

\[
h_{jk\ell} = \sum_{i=1}^{N_j} d_{jk}(t_i) H_{j\ell}(t_i). \tag{21.45}
\]

Completing the square in Eq. (21.44), one obtains:

\[
P(U_j|DI) \propto \int \prod_{l=1}^{v_jk} \mathcal{P}(\omega_{jk\ell}|I) \prod_{k=1}^n \left[ \frac{1}{\sigma_k} \left( 2\pi \sigma_k^2 \right)^{-\frac{N_k+u_j}{2}} \gamma^{-\frac{N_k+u_j}{2}} \sum_{u_j} g_{j1} \cdots g_{ju_j} u_j \lambda_1^{-\frac{1}{2}} \cdots \lambda_u^{-\frac{1}{2}} \right]
\]

\[
\times \exp \left\{ -\frac{1}{2\sigma_k^2} \left[ d_k^2 - h_{jk\ell}^2 + \sum_{\ell=1}^{u_j} (A_{jk\ell} - h_{jk\ell})^2 \right] \right\}
\]

\[
\times dA_{jk1} \cdots dA_{jk\nu_j} d\sigma_1 \cdots d\sigma_n d\Omega_j. \tag{21.46}
\]
Designating the integral over the amplitudes as \( I_j \) and isolating it, Eq. (21.46) can be written as:

\[
P(U_j|D) \propto \int \prod_{k=1}^{n} \left[ \frac{1}{\sigma_k} \left( 2\pi \sigma_k^2 \right)^{-\frac{N_k}{2}} \gamma_{j,k}^{u_j} g_{j,k}^{u_j} \prod_{l=1}^{v_j} P(\omega_{jl}|I) \right] \\
\times \exp \left\{ -\frac{1}{2\sigma_k^2} \left[ d_k^2 - h_{j,k\ell}^2 \right] \right\} \times I_j d\sigma_1 \cdots d\sigma_n d\Omega_j \\
\] (21.47)

where the amplitude integral is given by:

\[
I_j = \prod_{k=1}^{n} \int \exp \left\{ -\frac{1}{2\sigma_k^2} \sum_{\ell=1}^{u_j} (A_{j,k\ell} - h_{j,k\ell})^2 \right\} dA_{j,k1} \cdots dA_{j,ku_j}.
\] (21.48)

Introducing a change of variables

\[
z_{j,k\ell} = \frac{1}{\sqrt{2}\sigma_k} (A_{j,k\ell} - h_{j,k\ell})
\] (21.49)

with volume element given by

\[
\sqrt{2}\sigma_k dz_{j,k\ell} = dA_{j,k\ell}
\] (21.50)

the integral \( I_j \) becomes

\[
I_j = \int_{-\infty}^{\infty} \exp \left\{ -\sum_{\ell=1}^{u_j} z_{j,k\ell}^2 \right\} \sqrt{2}\sigma_k dz_{j,k1} \cdots \sqrt{2}\sigma_k dz_{j,ku_j}
\] (21.51)

\[
= (\sqrt{2}\sigma_k)^{u_j} \int_{-\infty}^{\infty} \exp \left\{ -\sum_{\ell=1}^{u_j} z_{j,k\ell}^2 \right\} dz_{j,k1} \cdots dz_{j,ku_j}
\]

\[
= (\sqrt{2}\sigma_k)^{u_j} (\sqrt{\pi})^{u_j}
\]

\[
= (2\pi \sigma_k^2)^{\frac{u_j}{2}}.
\]

Inserting \( I_j \) back into Eq. (21.47), the posterior probability for model \( U_j \) is given by

\[
P(U_j|D) \propto \int \prod_{k=1}^{n} \left[ \frac{1}{\sigma_k} \left( 2\pi \sigma_k^2 \right)^{-\frac{N_k}{2}} \gamma_{j,k}^{u_j} g_{j,k}^{u_j} \prod_{l=1}^{v_j} P(\omega_{jl}|I) \right] \\
\times \exp \left\{ -\frac{1}{2\sigma_k^2} \left[ d_k^2 - h_{j,k\ell}^2 \right] \right\} d\sigma_1 \cdots d\sigma_n d\Omega_j.
\] (21.52)

The reason for the unusual functional form for the prior probability for the amplitudes, Eq. (21.32), is that all of the pesky little values of \( 2\pi \) drop out and leave one with a much cleaner functional form for the posterior probability for the model.
21.1.2.2 Marginalizing The Noise Standard Deviation

To evaluate the integrals over the \( \sigma_k \), the integrand must be rearranged to isolate the integral:

\[
P(U_j | DI) \propto \prod_{k=1}^{n} \left[ \gamma_{u_j} g_{j11} \cdots g_{ju_j u_j} \left( \prod_{l=1}^{v_j} P(\omega_{jl} | I) \right) \right] \prod_{k=1}^{n} \left[ \frac{\lambda_1^{\frac{1}{2}} \cdots \lambda_{u_j}^{\frac{1}{2}}}{\lambda_1^{\frac{1}{2}} \cdots \lambda_{u_j}^{\frac{1}{2}}} \right] \left[ \int \int_{\sigma_k} \frac{1}{\sigma_k} \left( \frac{2\pi \sigma_k^2}{N_k^2} \right)^{-\frac{N_k}{2}} \exp \left\{ -\frac{1}{2\sigma_k^2} \left[ d_k^2 - h_{jk}^2 \right] \right\} d\sigma_1 \cdots d\sigma_n d\Omega_j \right].
\]

(21.53)

All of the integrals over the \( \sigma_k \) have the same functional form, so we can evaluate one of these integrals and then use the results to evaluate the remaining integrals. Evaluating the integral over \( \sigma_k \) one has

\[
I_{\sigma_k} = \int_0^{\infty} \frac{1}{\sigma_k} \left( \frac{2\pi \sigma_k^2}{N_k^2} \right)^{-\frac{N_k}{2}} \exp \left\{ -\frac{1}{2\sigma_k^2} \left[ d_k^2 - h_{jk}^2 \right] \right\} d\sigma_k
\]

(21.54)

and introducing the notation

\[
Q_{jk} = \frac{1}{2} \left[ d_k^2 - h_{jk}^2 \right]
\]

(21.55)

and \( I_{\sigma_k} \) becomes

\[
I_{\sigma_k} = (2\pi)^{-\frac{N_k}{2}} \int_0^{\infty} \sigma_k^{-(N_k+1)} \exp \left\{ -\frac{Q_{jk}}{\sigma_k^2} \right\} d\sigma_k
\]

(21.56)

This integral can be transformed into a Gamma function. A gamma function is defined as:

\[
\Gamma(z) = \int_0^{\infty} t^{z-1} \exp(-t) dt
\]

(21.57)

so a simple change of variables and a little algebra and the integral \( I_{\sigma_k} \) is then given by

\[
I_{\sigma_k} = \left[ \frac{1}{2} \Gamma \left( \frac{N_k}{2} \right) \right] \left( 2\pi Q_{jk} \right)^{-\frac{N_k}{4}}
\]

(21.58)

Inserting Eq. (21.58) into Eq. (21.53) one obtains

\[
P(U_j | DI) \propto \prod_{l=1}^{v_j} P(\omega_{jl} | I) \prod_{k=1}^{n} \left[ \gamma_{u_j} g_{j11} \cdots g_{ju_j u_j} \left( \prod_{l=1}^{v_j} P(\omega_{jl} | I) \right) \right] \left[ \Gamma \left( \frac{N_k}{2} \right) \right] \left( 2\pi Q_{jk} \right)^{-\frac{N_k}{4}} d\Omega_j.
\]

(21.59)

as the posterior probability for the model where we dropped the factor of one half, because it is exactly the same for all of the \( P(U_j | DI) \) and so cancels when this distribution is normalized.

This equation is correct, but not very computationally convenient because it requires an eigenvalue decomposition every time one evaluates the posterior probability. Fortunately, there are a few modifications that can be done that improve computational efficiency significantly without making approximations. First, note the presence of the eigenvalues, they are simply the determinant of the \( g_{jlm} \) matrix and can be computed with a matrix inverse. Making this substitution one obtains

\[
P(U_j | DI) \propto \prod_{l=1}^{v_j} P(\omega_{jl} | I) \prod_{k=1}^{n} \left[ \gamma_{u_j} g_{j11} \cdots g_{ju_j u_j} \left| g_{jlm} \right|^{-\frac{1}{2}} \right] Q_{jk}^{-\frac{N_k}{4}} d\Omega_j.
\]

(21.60)
Next the function $Q_{jk}$ can be computed using a matrix inverse instead of an eigenvalue decomposition, thus supplying the determinate mentioned earlier as well as allowing evaluation of the $Q_{jk}$ function. The integral over an amplitude in a Gaussian quadrature integral, just constrains the amplitudes to their maximum posterior probability values. Consequently, we can write

$$Q_{jk} = \sum_{i=1}^{N_j} \left[ d_k(t_i) - \sum_{l=1}^{u_j} \hat{B}_{jl} G_{jl}(t_i, \Omega_j) \right]^2$$  \hspace{1cm} (21.61)$$

and its mathematically the same as doing the eigenvalue decomposition. The amplitudes in this equation, the $\hat{B}_{jl}$, are given by the solution to

$$\sum_{k=1}^{v} g_{jk\ell} \hat{B}_{j\ell} = T_{j\ell}.$$ \hspace{1cm} (21.62)$$

The right-hand side of this equation is the projection of the data onto the model components and is given by

$$T_{j\ell} = \sum_{i=1}^{N_j} d_j(t_i) G_{j\ell}(t_i).$$ \hspace{1cm} (21.63)$$

See [2], and [11] for more on how the integrals over the amplitudes are evaluated.

Equation 21.60 is the joint posterior probability for the nonlinear parameters and is targeted by the Markov chain Monte Carlo simulations used to evaluate the remaining integrals. 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. (21.62). 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.

## 21.2 Outputs Form The Enter Ascii Model Package

The Text outputs files from the Enter Ascii Model Selection packages consist of: “Bayes.prob.model,” “BayesModelAscii.mcmc.values,” “Bayes.params,” “Console.log,” “Bayes.accepted” and a condensed file “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

$$\text{ModelFileName.ParamName}$$

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:

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

\begin{verbatim}
MyFunnyExp.FunnyDecayTime
\end{verbatim}

containing the posterior probability for the decay time. For more on writing Ascii models in either Fortran or C, see Appendix E.
Bibliography


[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.


