Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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Appendix D

McMC Values Report

The McMC Values report is the main output report from the various packages that run Markov chain Monte Carlo simulations. The report consists of three parts, the first part is shown in Fig. D.1. This part of the report is essentially a listing of the parameter file that was used when the package was run. These parameters consist of the various parameter settings used to control the Markov chain Monte Carlo simulations, the top part of this listing. The middle part consists of the information about the various prior probabilities and finally the bottom part of the parameter file is any configuration parameters that are set for this particular package. The parameter listings at the top of Fig. D.1 are standardized across all packages. Additionally, when prior probabilities are show, there format is also standardized. For those looking closely at this figure, you may notice that I have reformed this first part of the report to get it to paginate correctly.

The middle part of the Mcmc Values report is shown in Fig. D.2. The middle part of the Mcmc Values report lists the simulation that had maximum posterior probability. Since simulations are essentially defined by their posterior probabilities, the first part of this report shown the posterior probability, the likelihood and the prior probability. The NonLinear parameter estimates are just the parameters that had maximum posterior probability. Note that this is a listing of the parameters which were actually used in the Markov chain Monte Carlo simulation. For packages that use marginalization, beneath the nonlinear parameters are the estimated amplitudes. For packages that do not use marginalization, but treat amplitudes like nonlinear parameters, this section does not occur. When multiple data sets are processed these amplitudes will be repeated one time for each data set. Finally, the last part of this center section is the estimated noise standard deviation for each data set.

The last part of the Mcmc Values report is shown in Fig. D.3. The bottom part of the Mcmc Values report is the heart of this report. Before I discuss the parameter estimates, I want to draw your attention to the top part of this lower section, Fig. D.3, in particular the line containing “Log probability for the Model:”; This line is the expected logarithm of the likelihood computed using thermodynamic integration, see Chapter C for more on how this number is computed. It contains the mean and standard deviation parameter estimates. Each nonlinear parameter is listed at the front. These nonlinear parameters are followed by the amplitudes, and then the estimated noise standard deviation for each data set. The mean values estimates are computed by averaging the value of a parameter from all of the Markov chain Monte Carlo simulations. Similarly, the standard deviation is the standard deviation of the parameter estimates taken from all Markov chain Monte Carlo simulations.
Figure D.1: The McMC Values Report Header

Parameter File Listing for the Given Exponential package

! BayesExpGiven Package
! Created 03-Oct-2011 16:21:18 by larry
!
  Output Dir = BayesOtherAnalysis
  Number Of Abscissa = 1
  Number Of Columns = 1
  Number Of Sets = 1
    File Name = BayesOtherAnalysis/001.dat
  McMC Simulations = 96
  McMC Repeats = 30
  Total Mcmc Samples = 2880
  Kill Count = 9
  Minimum Annealing Steps = 101
  Histogram Type = Binned
  Outlier Detection = Disabled
  Number Of Priors = 3

  Param Name      Low       Mean       High       Std Dev      Norm  Prior  Ordered Param Type
  Rate             0.000E+00 0.000E+00 2.432E+00 8.109E-01 -3.7417E+00 Gaussian LowHigh NonLinear
  Amplitude       -1.000E+06 0.000E+00 1.000E+06 3.000E+05 -3.6262E+00 Gaussian NotOrdered Amplitude
  Constant        -1.000E+06 0.000E+00 1.000E+06 3.000E+05 -3.6262E+00 Gaussian NotOrdered Amplitude

Package Parameters = 2
  Number of Exp = 2
  Constant = YES

Figure D.1: The McMC Value report is the main report from packages that run Markov chain Monte Carlo simulations. The report consists of three parts, the first part is shown here. This part of the report is essentially a listing of the parameter file that was used when the package was run. These parameters consists of the various parameter settings used to control the Markov chain Monte Carlo simulations, the top part of this listing. The middle part consists of the information about the various prior probabilities and finally the bottom part of the parameter file is any configuration parameters that are set for this particular package.
McMC Values Report for the Given Exponential Package (2 Exp with a Constant)

-------------- Simulation With Maximum Posterior Probability --------------

Probability:  -0.11967275E+03
Likelihood:  -0.10055787E+03
Prior:  -0.19114882E+02
Number of Parameters:  2
Number of Derived:  2
Number of Model Vectors:  3
Number of Outliers:  0
Number of Sets:  1

NonLinear Parameter Estimates

<table>
<thead>
<tr>
<th>Param#</th>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Rate_1</td>
<td>1.42948109E-04</td>
</tr>
<tr>
<td>2</td>
<td>Rate_2</td>
<td>9.95064682E-01</td>
</tr>
</tbody>
</table>

Amplitude Estimate, (Peak Posterior)

<table>
<thead>
<tr>
<th>Set#</th>
<th>Amp%</th>
<th>Amplitude_Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>Amplitude_1</td>
<td>3.75907093E+01</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>Amplitude_2</td>
<td>-1.25075235E+02</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>Constant</td>
<td>3.76596504E+01</td>
</tr>
</tbody>
</table>

Derived Parameters Estimates

<table>
<thead>
<tr>
<th>Derived#</th>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Time_1</td>
<td>6.99554652E+03</td>
</tr>
<tr>
<td>2</td>
<td>Time_2</td>
<td>1.00495980E+00</td>
</tr>
</tbody>
</table>

Noise Std Dev Estimates By Set

<table>
<thead>
<tr>
<th>NoiseStdDev#</th>
<th>Name, Set</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NoiseStdDev, Set 1</td>
<td>7.71617382E-01</td>
</tr>
</tbody>
</table>

-------------- End Simulation With Maximum Posterior Probability --------------

Figure D.2: This is the back or bottom part of the mcmc values report generated by the Bayes Test Data package. This part of the report consists of an image mask. This mask is one byte per pixel with the horizontal axis being the readout direction and the vertical part being the phase encode. The locations of the ones are the pixels that have a signal, the zero pixels have noise but no signal. So the first nonzero pixel is curve of 2 and ro of 5. If you look at the list of slices at the bottom the first output is pe=2 and ro=5, the numerical values are the actual values used by the program to generate this pixel.
Figure D.3: The McMC Values Report, The End

<table>
<thead>
<tr>
<th>Parameter Description</th>
<th>Mean Value</th>
<th>Std. Dev.</th>
<th>Peak Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rate_1</td>
<td>6.70911E-01</td>
<td>2.77481E-01</td>
<td>1.42948E-04</td>
</tr>
<tr>
<td>Rate_2</td>
<td>1.08244E+00</td>
<td>1.41600E-01</td>
<td>9.95065E-01</td>
</tr>
<tr>
<td>Time_1</td>
<td>6.61852E+00</td>
<td>1.35603E+02</td>
<td>6.99555E+03</td>
</tr>
<tr>
<td>Time_2</td>
<td>9.35569E-01</td>
<td>9.17764E-02</td>
<td>1.00496E+00</td>
</tr>
<tr>
<td>Amplitude_1, Set 1</td>
<td>-3.53161E+01</td>
<td>3.61905E+01</td>
<td>3.75907E+01</td>
</tr>
<tr>
<td>Amplitude_2, Set 1</td>
<td>-8.97797E+01</td>
<td>3.59562E+01</td>
<td>-1.25075E+02</td>
</tr>
<tr>
<td>Constant, Set 1</td>
<td>7.52243E+00</td>
<td>2.39747E+00</td>
<td>3.76597E+01</td>
</tr>
<tr>
<td>AmpRms.Set.1</td>
<td>1.31971E+02</td>
<td>1.25815E+01</td>
<td>1.35923E+02</td>
</tr>
<tr>
<td>NoiseStdDev, Set 1</td>
<td>7.80983E-01</td>
<td>9.35638E-03</td>
<td>7.71617E-01</td>
</tr>
</tbody>
</table>

The expected parameter values (mean value of the probability distributions):

The Average Log Posterior Probability Was: -122.3195  1.04559
The Average Log Prior Params: -19.6689  0.46091
The Average Log Likelihood:  -102.6507  0.95375
Log Probability for the Model:  -105.1542

Figure D.3: The bottom part of the Mcmc Values report is the heart of this report. It contains the mean and standard deviation parameter estimates. Each nonlinear parameter is listed at the front. These nonlinear parameters are followed by the amplitudes, and then the estimated noise standard deviation for each data set. The mean values estimates are computed by averaging the value of a parameter from all of the Markov chain Monte Carlo simulations. Similarly, the standard deviation is the standard deviation of the parameter estimates taken from all Markov chain Monte Carlo simulations. The Peak Value is just a repeat of what is shown in the center section of this report and is shown for informational purposes.
Carlo simulations. The Peak Value is just a repeat of what is shown in the center section of this report and is shown for informational purposes.

The McMC values report is meant as a kind of summary of every important aspect of the analysis. As noted the first part of this report contains the setup information. This information includes things like the number of Markov chain simulations run, the number of repeats gathered, the total number of samples gathered and the minimum number of annealing steps. The middle part of the report is a print out of the simulation that had maximum posterior probability. This print out includes probabilities, posterior, prior and likelihood and it includes the parameters that had maximum posterior probability. Note that Markov chain Monte Carlo simulations explore the posterior probability, they do not actually locate the maximum. Consequently, the parameters printed in this section are strictly the parameters that had maximum posterior for all of the simulations gathered in the analysis; they are not strictly the parameters that maximized the posterior. The bottom part of this report contains the mean and standard deviation parameter estimates and it contains an estimate and standard deviation of the various probabilities. Finally, it also includes the expected value of the logarithm of the likelihood. Because each model in each Ascii package is different, this section of the report varies from package to package, and in the case of the Ascii Model packages the report varies with the loaded model. Finally, the bottom part of this report contains the mean and standard deviation estimates.
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 American Institute of Physics and if you do not have access to Science Sitations you many not be able to retrieve this paper.


