

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

October 21, 2016

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
21 Enter Ascii Model Selection	337
21.1 The Bayesian Calculations	339
21.1.1 The Direct Probability With No Amplitude Marginalization	340
21.1.2 The Direct Probability With Amplitude Marginalization	342
21.1.2.1 Marginalizing the Amplitudes	343
21.1.2.2 Marginalizing The Noise Standard Deviation	348

21.2	Outputs Form The Enter Ascii Model Package	349
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
21.1	The Enter Ascii Model Selection Package Interface	338

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 28

Analyze Image Pixel

The Analyze Image Pixel package allows you to enter a model of your own and then use Bayesian probability theory to analyze that model.¹ The Java interface to the Image Pixel package is shown in Fig. 28.1. The Bayesian calculations performed by this package are identical to those in Bayes Enter Ascii, Chapter 20, and consequently we are not going to repeat those calculation here; rather in this Chapter we will concentrate our attention on the problem of how to use this package. To use this package, you must do the following:

Select the “Analyze Image Pixel” package from the Package menu.

Load the image data that is to be processed by the package. The analyze image Pixel package analyzes arrayed images on a pixel by pixel basis.

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

Load an abscissa file. A typical arrayed image data set is a stack of images each gathered at some parameter settings. For example, if the data are diffusion tensor data, then the abscissa would be a vector specifying the b values for each element in the array. These b values would be b_x , b_y and b_z . So the abscissa file would be a three column Ascii file containing the b values each element in the array. In general the user specifies the number of abscissa columns, See Chapter A.3 for more on the abscissa file. Note the Analyze Image Pixel package uses the same abscissa for every pixel in the data.

Build the model using the “Build” button.

Check the Analysis Options boxes as you see fit.

Find Outliers tells the package to use an outlier model to select and eliminate pixels with odd characteristics.

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 28.1: The Interface To The Analyze Image Pixels Package

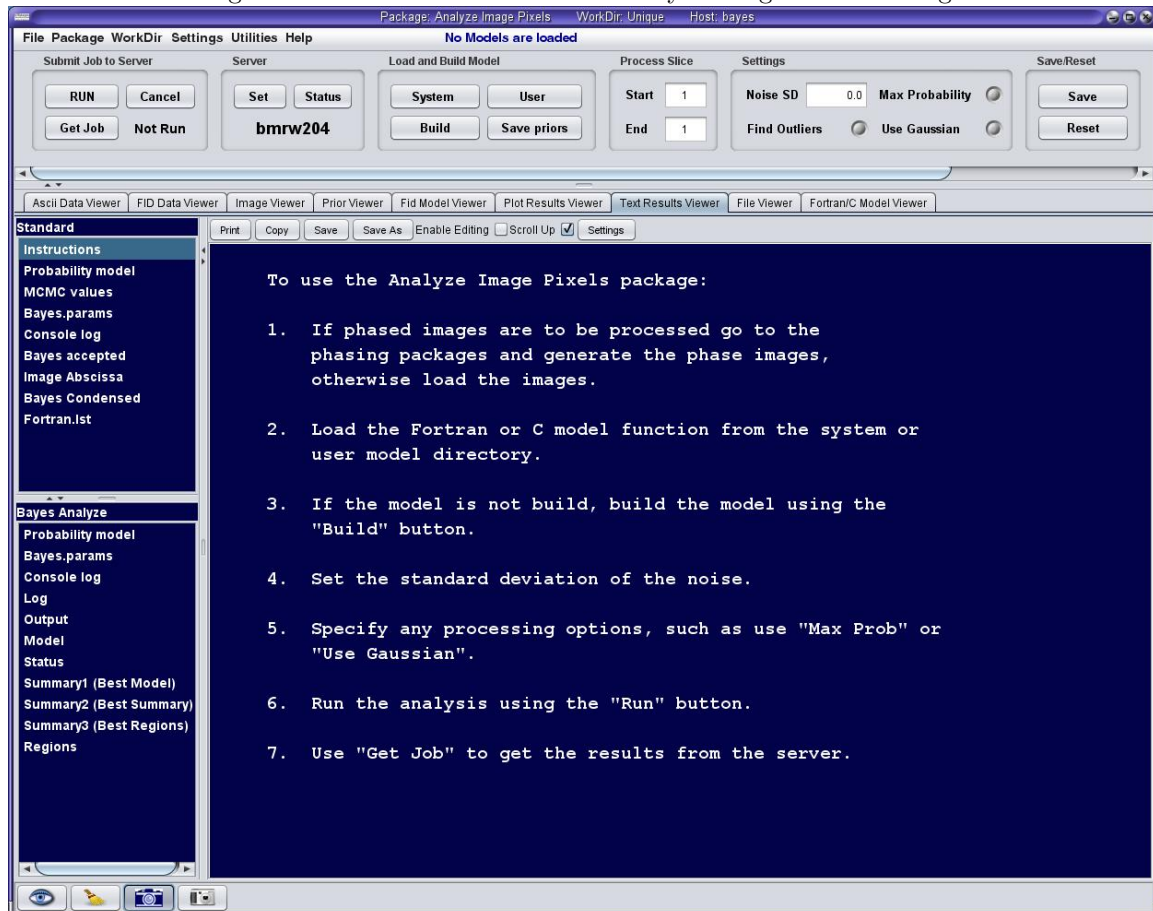


Figure 28.1: The Analyze Image Pixel package allows the user to load an arrayed image and then load a model, either system defined or user defined, and analyze the input image on a pixel by pixel basis using the loaded model. Prior to running an analysis, you must also load an appropriate Abcissa file. Unlike Ascii input data, which requires an Abcissa to load, any image can be loaded. So to process the data the Abcissa values must be loaded.

Max Probability tells the package to locate the maximum of the posterior probability. Locating the maximum is done using a searching algorithm and is much faster than using a Markov chain Monte Carlo algorithm. When Max Probability is selected the output images are generated using the parameters that maximized the posterior probability.

Use Gaussian tells the package to switch from using a t -distribution to using a Gaussian. In this case the input standard deviation of the noise is used as the standard deviation of the Gaussian likelihood. If Use Gaussian is not selected, a Student's t -distribution is used for the likelihood. The input noise standard deviation is used to threshold pixels. Arrays of pixels having a root mean-square smaller than the input standard deviation of the noise are not processed.

Set the Noise SD to a value equal to your best estimate of the standard deviation of the noise in the image stack that is to be processed. To get an estimate of the noise standard deviation, draw an ROI in a region where there is no signal and hit the "Get Statistics" button. The output on the right-hand side labeled "RMS" contains the root mean-square image pixel value and is a good estimate of the noise standard deviation.

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.

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.

The actual processing done by this package are essentially the same as that done in the Bayes Enter Ascii package and we refer you to that package, Chapter 20, for more on the processing being done. However, there is one difference: the Analyze Image Pixel package does a model selection calculation. In this calculation there are two models: a No Signal model, and a signal model. The No Signal model assumes the signal consists of only noise while the signal model assumes the signal is given by your model plus noise. When the no signal model is selected, there are no output parameters. Output parameter maps contain zero in these no signal regions. However, there is an exception to this, on the output map containing the standard deviation of the noise, both signal and no signal regions have an estimate of the noise standard deviation. In regions with no signal, the standard deviation is computed as the root mean-square of the total data value. In regions containing signals, the output standard deviation is computed as the root means-square residual.

28.1 Modification History

In release 4.10, the Markov chain Monte Carlo routine in Bayes Image Pixels was replaced by one as similar to the one in the Enter Ascii Model package, Chapter 20, as possible. This was done because in some cases the Enter Ascii package's Markov chain was able to solve problems that Bayes Image Pixel package could not. Given that the data and the model were identical in the cases at hand, I

concluded the Markov chain in Bayes Image Pixels package needed replacing. The new routine is almost line by line identical to the routine in the Enter Ascii package.

In addition to replacing the Markov chain, I also modified the output routines so that it tests each output image to see if it is null, i.e., all zero. If the image is zero everywhere nothing is written. This was done to eliminate a perceived problem. In the process of testing a new model, a user generated an image containing no signal and then ran the Bayes Image Pixel using the no signal image and his new model. The old Bayes Image Pixel package correctly identified the pixels as no signal and so set the output images to zero. When processing was complete, the output routines wrote these zero images, and the users, myself included, interpreted these zero output images as an error on the part of Bayes Image Pixels package. That interpretation was incorrect and as soon as I realized what was happening, I modified the output routines so that zero images are not written.

Bibliography

- [1] Rev. Thomas Bayes (1763), “An Essay Toward Solving a Problem in the Doctrine of Chances,” *Philos. Trans. R. Soc. London*, **53**, pp. 370-418; reprinted in *Biometrika*, **45**, pp. 293-315 (1958), and *Facsimiles of Two Papers by Bayes*, with commentary by W. Edwards Deming, New York, Hafner, 1963.
- [2] G. Larry Bretthorst (1988), “Bayesian Spectrum Analysis and Parameter Estimation,” in *Lecture Notes in Statistics*, **48**, J. Berger, S. Fienberg, J. Gani, K. Krickenberg, and B. Singer (eds), Springer-Verlag, New York, New York.
- [3] G. Larry Bretthorst (1990), “An Introduction to Parameter Estimation Using Bayesian Probability Theory,” in *Maximum Entropy and Bayesian Methods*, Dartmouth College 1989, P. Fougère ed., pp. 53-79, Kluwer Academic Publishers, Dordrecht the Netherlands.
- [4] G. Larry Bretthorst (1990), “Bayesian Analysis I. Parameter Estimation Using Quadrature NMR Models” *J. Magn. Reson.*, **88**, pp. 533-551.
- [5] G. Larry Bretthorst (1990), “Bayesian Analysis II. Signal Detection And Model Selection” *J. Magn. Reson.*, **88**, pp. 552-570.
- [6] G. Larry Bretthorst (1990), “Bayesian Analysis III. Examples Relevant to NMR” *J. Magn. Reson.*, **88**, pp. 571-595.
- [7] G. Larry Bretthorst (1991), “Bayesian Analysis. IV. Noise and Computing Time Considerations,” *J. Magn. Reson.*, **93**, pp. 369-394.
- [8] G. Larry Bretthorst (1992), “Bayesian Analysis. V. Amplitude Estimation for Multiple Well-Separated Sinusoids,” *J. Magn. Reson.*, **98**, pp. 501-523.
- [9] G. Larry Bretthorst (1992), “Estimating The Ratio Of Two Amplitudes In Nuclear Magnetic Resonance Data,” in *Maximum Entropy and Bayesian Methods*, C. R. Smith et al. (eds.), pp. 67-77, Kluwer Academic Publishers, the Netherlands.
- [10] G. Larry Bretthorst (1993), “On The Difference In Means,” in *Physics & Probability Essays in honor of Edwin T. Jaynes*, W. T. Grandy and P. W. Milonni (eds.), pp. 177-194, Cambridge University Press, England.
- [11] G. Larry Bretthorst (1996), “An Introduction To Model Selection Using Bayesian Probability Theory,” in *Maximum Entropy and Bayesian Methods*, G. R. Heidbreder, ed., pp. 1-42, Kluwer Academic Publishers, Printed in the Netherlands.

- [12] G. Larry Bretthorst (1999), “The Near-Irrelevance of Sampling Frequency Distributions,” in *Maximum Entropy and Bayesian Methods*, W. von der Linden *et al.* (eds.), pp. 21-46, Kluwer Academic Publishers, the Netherlands.
- [13] G. Larry Bretthorst (2001), “Nonuniform Sampling: Bandwidth and Aliasing,” in *Maximum Entropy and Bayesian Methods in Science and Engineering*, Joshua Rychert, Gary Erickson and C. Ray Smith *eds.*, pp. 1-28, American Institute of Physics, USA.
- [14] G. Larry Bretthorst, Christopher D. Kroenke, and Jeffrey J. Neil (2004), “Characterizing Water Diffusion In Fixed Baboon Brain,” in *Bayesian Inference And Maximum Entropy Methods In Science And Engineering*, Rainer Fischer, Roland Preuss and Udo von Toussaint *eds.*, AIP conference Proceedings, **735**, pp. 3-15.
- [15] G. Larry Bretthorst, William C. Hutton, Joel R. Garbow, and Joseph J.H. Ackerman (2005), “Exponential parameter estimation (in NMR) using Bayesian probability theory,” *Concepts in Magnetic Resonance*, 27A, Issue 2, pp. 55-63.
- [16] G. Larry Bretthorst, William C. Hutton, Joel R. Garbow, and Joseph J. H. Ackerman (2005), “Exponential model selection (in NMR) using Bayesian probability theory,” *Concepts in Magnetic Resonance*, 27A, Issue 2, pp. 64-72.
- [17] G. Larry Bretthorst, William C. Hutton, Joel R. Garbow, and Joseph J.H. Ackerman (2005), “How accurately can parameters from exponential models be estimated? A Bayesian view,” *Concepts in Magnetic Resonance*, 27A, Issue 2, pp. 73-83.
- [18] G. Larry Bretthorst, W. C. Hutton, J. R. Garbow, and Joseph J. H. Ackerman (2008), “High Dynamic Range MRS Time-Domain Signal Analysis,” *Magn. Reson. in Med.*, **62**, pp. 1026-1035.
- [19] V. Chandramouli, K. Ekberg, W. C. Schumann, S. C. Kalhan, J. Wahren, and B. R. Landau (1997), “Quantifying gluconeogenesis during fasting,” *American Journal of Physiology*, **273**, pp. H1209-H1215.
- [20] R. T. Cox (1961), “The Algebra of Probable Inference,” Johns Hopkins Univ. Press, Baltimore.
- [21] André d’Avignon, G. Larry Bretthorst, Marlyn Emerson Holtzer, and Alfred Holtzer (1998), “Site-Specific Thermodynamics and Kinetics of a Coiled-Coil Transition by Spin Inversion Transfer NMR,” *Biophysical Journal*, **74**, pp. 3190-3197.
- [22] André d’Avignon, G. Larry Bretthorst, Marlyn Emerson Holtzer, and Alfred Holtzer (1999), “Thermodynamics and Kinetics of a Folded-Folded Transition at Valine-9 of a GCN4-Like Leucine Zipper,” *Biophysical Journal*, **76**, pp. 2752-2759.
- [23] David Freedman, and Persi Diaconis (1981), “On the histogram as a density estimator: L_2 theory,” *Zeitschrift für Wahrscheinlichkeitstheorie und verwandte Gebiete*, **57**, 4, pp. 453-476.
- [24] W. R. Gilks, S. Richardson, and D. J. Spiegelhalter (1996), “Markov Chain Monte Carlo in Practice,” Chapman & Hall, London.

- [25] Paul M. Goggans, and Ying Chi (2004), “Using Thermodynamic Integration to Calculate the Posterior Probability in Bayesian Model Selection Problems,” in *Bayesian Inference and Maximum Entropy Methods in Science and Engineering: 23rd International Workshop*, **707**, pp. 59-66.
- [26] Marlyn Emerson Holtzer, G. Larry Bretthorst, D. André d’Avignon, Ruth Hogue Angelette, Lisa Mints, and Alfred Holtzer (2001), “Temperature Dependence of the Folding and Unfolding Kinetics of the GCN4 Leucine Lipper via ^{13}C alpha-NMR,” *Biophysical Journal*, **80**, pp. 939-951.
- [27] E. T. Jaynes (1968), “Prior Probabilities,” *IEEE Transactions on Systems Science and Cybernetics*, SSC-4, pp. 227-241; reprinted in [30].
- [28] E. T. Jaynes (1978), “Where Do We Stand On Maximum Entropy?” in *The Maximum Entropy Formalism*, R. D. Levine and M. Tribus *Eds.*, pp. 15-118, Cambridge: MIT Press, Reprinted in [30].
- [29] E. T. Jaynes (1980), “Marginalization and Prior Probabilities,” in *Bayesian Analysis in Econometrics and Statistics*, A. Zellner *ed.*, North-Holland Publishing Company, Amsterdam; reprinted in [30].
- [30] E. T. Jaynes (1983), “Papers on Probability, Statistics and Statistical Physics,” a reprint collection, D. Reidel, Dordrecht the Netherlands; second edition Kluwer Academic Publishers, Dordrecht the Netherlands, 1989.
- [31] E. T. Jaynes (1957), “How Does the Brain do Plausible Reasoning?” unpublished Stanford University Microwave Laboratory Report No. 421; reprinted in *Maximum-Entropy and Bayesian Methods in Science and Engineering* **1**, pp. 1-24, G. J. Erickson and C. R. Smith *Eds.*, 1988.
- [32] E. T. Jaynes (2003), “Probability Theory—The Logic of Science,” edited by G. Larry Bretthorst, Cambridge University Press, Cambridge UK.
- [33] Sir Harold Jeffreys (1939), “Theory of Probability,” Oxford Univ. Press, London; Later editions, 1948, 1961.
- [34] John G. Jones, Michael A. Solomon, Suzanne M. Cole, A. Dean Sherry, and Craig R. Malloy (2001) “An integrated ^2H and ^{13}C NMR study of gluconeogenesis and TCA cycle flux in humans,” *American Journal of Physiology, Endocrinology, and Metabolism*, **281**, pp. H848-H856.
- [35] John Kotyk, N. G. Hoffman, W. C. Hutton, G. Larry Bretthorst, and J. J. H. Ackerman (1992), “Comparison of Fourier and Bayesian Analysis of NMR Signals. I. Well-Separated Resonances (The Single-Frequency Case),” *J. Magn. Reson.*, **98**, pp. 483–500.
- [36] Pierre Simon Laplace (1814), “A Philosophical Essay on Probabilities,” John Wiley & Sons, London, Chapman & Hall, Limited 1902. Translated from the 6th edition by F. W. Truscott and F. L. Emory.
- [37] N. Lartillot, and H. Philippe (2006), “Computing Bayes Factors Using Thermodynamic Integration,” *Systematic Biology*, **55** (2), pp. 195-207.

- [38] D. Le Bihan, and E. Breton (1985), “Imagerie de diffusion in-vivo par rsonance,” Comptes rendus de l’Acadmie des Sciences (Paris), **301** (15), pp. 1109-1112.
- [39] N. R. Lomb (1976), “Least-Squares Frequency Analysis of Unevenly Spaced Data,” *Astrophysical and Space Science*, **39**, pp. 447-462.
- [40] T. J. Loredo (1990), “From Laplace To SN 1987A: Bayesian Inference In Astrophysics,” in *Maximum Entropy and Bayesian Methods*, P. F. Fougere (ed), Kluwer Academic Publishers, Dordrecht, The Netherlands.
- [41] Craig R. Malloy, A. Dean Sherry, and Mark Jeffrey (1988), “Evaluation of Carbon Flux and Substrate Selection through Alternate Pathways Involving the Citric Acid Cycle of the Heart by ^{13}C NMR Spectroscopy,” *Journal of Biological Chemistry*, **263** (15), pp. 6964-6971.
- [42] Craig R. Malloy, Dean Sherry, and Mark Jeffrey (1990), “Analysis of tricarboxylic acid cycle of the heart using ^{13}C isotope isomers,” *American Journal of Physiology*, **259**, pp. H987-H995.
- [43] Lawrence R. Mead and Nikos Papanicolaou, “Maximum entropy in the problem of moments,” *J. Math. Phys.* **25**, 2404–2417 (1984).
- [44] K. Merboldt, Wolfgang Hanicke, and Jens Frahm (1969), “Self-diffusion NMR imaging using stimulated echoes,” *Journal of Magnetic Resonance*, **64** (3), pp. 479-486.
- [45] Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller (1953), “Equation of State Calculations by Fast Computing Machines,” *Journal of Chemical Physics*. The previous link is to the Americain Institute of Physics and if you do not have access to Science Sitations you many not be able to retrieve this paper.
- [46] Radford M. Neal (1993), “Probabilistic Inference Using Markov Chain Monte Carlo Methods,” technical report CRG-TR-93-1, Dept. of Computer Science, University of Toronto.
- [47] Jeffrey J. Neil, and G. Larry Bretthorst (1993), “On the Use of Bayesian Probability Theory for Analysis of Exponential Decay Data: An Example Taken from Intravoxel Incoherent Motion Experiments,” *Magn. Reson. in Med.*, **29**, pp. 642–647.
- [48] H. Nyquist (1924), “Certain Factors Affecting Telegraph Speed,” *Bell System Technical Journal*, **3**, pp. 324-346.
- [49] H. Nyquist (1928), “Certain Topics in Telegraph Transmission Theory,” *Transactions AIEE*, **3**, pp. 617-644.
- [50] William H. Press, Saul A. Teukolsky, William T. Vetterling and Brian P. Flannery (1992), “Numerical Recipes The Art of Scientific Computing Second Edition,” Cambridge University Press, Cambridge UK.
- [51] Emanuel Parzen (1962), “On Estimation of a Probability Density Function and Mode,” *Annals of Mathematical Statistics* **33**, 1065–1076
- [52] Karl Pearson (1895), “Contributions to the Mathematical Theory of Evolution. II. Skew Variation in Homogeneous Material,” *Phil. Trans. R. Soc. A* **186**, 343–326.

- [53] Murray Rosenblatt, "Remarks on Some Nonparametric Estimates of a Density Function," *Annals of Mathematical Statistics* **27**, 832–837 (1956).
- [54] Jeffery D. Scargle (1981), "Studies in Astronomical Time Series Analysis I. Random Process In The Time Domain," *Astrophysical Journal Supplement Series*, **45**, pp. 1-71.
- [55] Jeffery D. Scargle (1982), "Studies in Astronomical Time Series Analysis II. Statistical Aspects of Spectral Analysis of Unevenly Sampled Data," *Astrophysical Journal*, **263**, pp. 835-853.
- [56] Jeffery D. Scargle (1989), "Studies in Astronomical Time Series Analysis. III. Fourier Transforms, Autocorrelation Functions, and Cross-correlation Functions of Unevenly Spaced Data," *Astrophysical Journal*, **343**, pp. 874-887.
- [57] Arthur Schuster (1905), "The Periodogram and its Optical Analogy," *Proceedings of the Royal Society of London*, **77**, p. 136-140.
- [58] Claude E. Shannon (1948), "A Mathematical Theory of Communication," *Bell Syst. Tech. J.*, **27**, pp. 379-423.
- [59] John E. Shore, and Rodney W. Johnson (1981), "Properties of cross-entropy minimization," *IEEE Trans. on Information Theory*, **IT-27**, No. 4, pp. 472-482.
- [60] John E. Shore and Rodney W. Johnson (1980), "Axiomatic derivation of the principle of maximum entropy and the principle of minimum cross-entropy," *IEEE Trans. on Information Theory*, **IT-26** (1), pp. 26-37.
- [61] Devinderjit Sivia, and John Skilling (2006), "Data Analysis: A Bayesian Tutorial," Oxford University Press, USA.
- [62] Edward O. Stejskal and Tanner, J. E. (1965), "Spin Diffusion Measurements: Spin Echoes in the Presence of a Time-Dependent Field Gradient." *Journal of Chemical Physics*, **42** (1), pp. 288-292.
- [63] D. G. Taylor and Bushell, M. C. (1985), "The spatial mapping of translational diffusion coefficients by the NMR imaging technique," *Physics in Medicine and Biology*, **30** (4), pp. 345-349.
- [64] Myron Tribus (1969), "Rational Descriptions, Decisions and Designs," Pergamon Press, Oxford.
- [65] P. M. Woodward (1953), "Probability and Information Theory, with Applications to Radar," McGraw-Hill, N. Y. Second edition (1987); R. E. Krieger Pub. Co., Malabar, Florida.
- [66] Arnold Zellner (1971), "An Introduction to Bayesian Inference in Econometrics," John Wiley and Sons, New York.