

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

475

Bibliography

479

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 11

Find Resonances

There are two frequency finding programs in the Bayesian Analysis Software: Bayes Analyze, Chapter 8, and Bayes Find Resonance. Bayes Analyze is a searching algorithm that uses the residuals from the current fit, to determine if there is evidence in the data for and additional resonance. While this procedure is implemented using Bayesian probability theory, it is still an approximation to computing the full Bayesian posterior probability for the number of resonances. We implemented Bayes Analyze in this way, so that it would be very fast. However, under some conditions, Bayes Analyze will miss resonances when they are either very close together or the signal-to-noise of the resonance is very low. To solve these problems, we implemented a frequency finding program that uses Markov chain Monte Carlo to compute the posterior probability for the number of resonances. The interface to the find resonance package is shown in Fig. 11.1 To use this package, you must do the following:

Select the Bayes Find Resonances package from the Package menu.

Load the Fid data that is to be analyzed. If the Fid is arrayed, select the trace that is to be analyzed. The trace analyzed is the currently displayed trace. At the present time only a single Fid is processed by Bayes Find Resonances package.

Select the phase model, the choices are correlated, uncorrelated and automatic.

- If the phase model is “Common,” the all resonances have the same phase.
- If the phase model is “Independent,” the all resonances have a different phase.
- If the phase model is “Automatic,” then the Bayes Find Resonances package computes the posterior probability for the phase of each resonance.

Check the “Constant” box if the data contains an offset.

Set the first and last Fids that are to be analyzed. Note that these Fids are analyzed separately, not jointly, so you will get an analysis for each selected Fid.

Set the maximum number of resonances that can be included in a model.

Select the server that is to process the analysis.

Figure 11.1: The Find Resonances Interface With The Ethyl Ether Spectrum

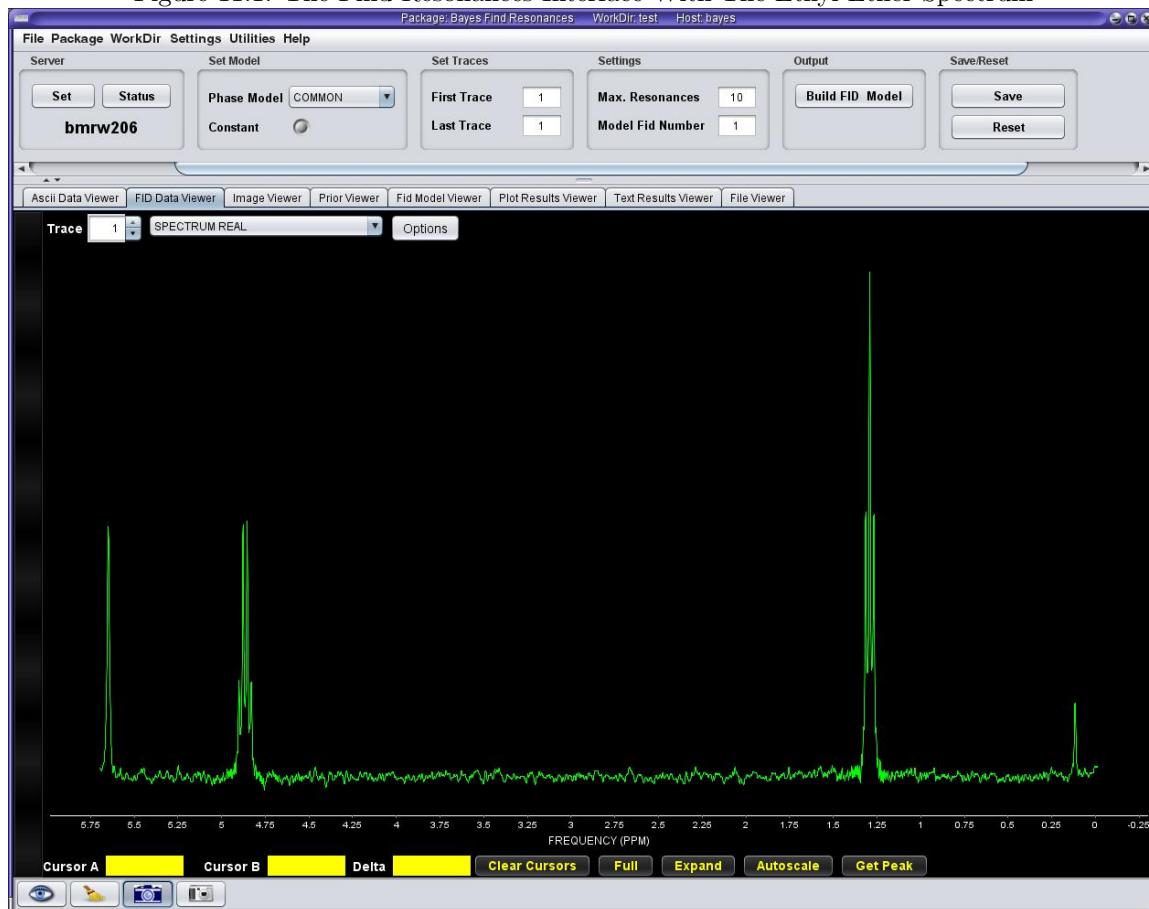


Figure 11.1: When the Find Resonances package is selected, this is the displayed interface. To use this package, load the Fid you wish to analyze. The spectrum of this Fid will be displayed in the Fid Data Viewer. Select the Fid you wish to analyze and display that Fid. At the present time only a single Fid may be processed at one time. Set the various optional feature of the model you wish to use and run the analysis. When the analysis finishes use the “Build Model” button to select and build a model of the Fid. The Fid Model Viewer can then be used to view this model.

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.

Unlike Bayes Analyze which outputs parameter estimates computed using the values that maximized the joint posterior probability for the parameters, Bayes Find Resonances outputs mean and standard deviation parameter estimates computed from all high probability models. That is to say if the probability for the number of resonances was 50% for 9 and 50% for 10 resonances, then there will be mean and standard deviation parameter estimates for the frequencies and decay rate constants from both of these models. Additionally, Bayes Find Resonances runs multiple Fids one right after the other. Consequently, when a Fid model of the time domain data is generated, you must specify both the resonance model and the number of the Fid to model. The Fid number to model is indicated using the “Model Fid Number” entry box. If there are multiples high probability resonance models, clicking on the “Build FID Model” button will show you a list of these models and you can select which one you wish to use in generating a time domain Fid model.

11.1 The Bayesian Calculations

The first step in all Bayesian calculations is to define the problem. Here, the problem is essentially a parameter estimation calculations where one is estimating the frequencies, amplitudes, decay rate constants and phases of multiple exponentially decaying sinusoidal. The model will designated as $\mathbf{M}(\mathbf{t}_i)$ where complex quantities will be in bold. Then symbolically the model which relates the complex data, model and noise is given by:

$$\mathbf{d}_i = \mathbf{M}(\mathbf{t}_i) + \mathbf{n}_i \quad (i \in \{1, \dots, N\}), \quad (11.1)$$

where N is the total number of complex data values, \mathbf{d}_i is a complex data values sampled at time t_i , and \mathbf{n}_i is a complex noise value at time t_i . The complex model $\mathbf{M}(\mathbf{t}_i)$ is given by:

$$\mathbf{M}(\mathbf{t}_i) = [\mathbf{F}\delta(t_i) + \mathbf{C}] \delta(\nu) + \sum_{j=1}^m A_j \exp \{2\pi i f_j(t_i - t_0) - \alpha_j t_i + i\phi\delta(\xi_j) + i\phi_j[1 - \delta(\xi_j)]\} \quad (11.2)$$

where \mathbf{F} is a model of the first data value, the function $\delta(\cdot)$ is defined below, \mathbf{C} is a complex offset, m is the unknown number of sinusoids, A_j is the amplitude of the j th sinusoid, f_j is the frequency of the j th sinusoid, t_0 is a first order phase correction, α_j is the decay rate constant of the j th sinusoid. The quantity “ $\phi\delta(\xi_j) + \phi_j[1 - \delta(\xi_j)]$ ” is the phase of the j sinusoid and is either a common zero order phase, ϕ , or a unique phase specific to the j th sinusoid, ϕ_j . Whether or not the phase is common or unique depends on the value of the indicator function $\delta(\xi_j)$. The indicator function $\delta(\cdot)$ is defined as

$$\delta(\nu) = \begin{cases} 1 & \text{If } \nu = 0 \\ 0 & \text{Otherwise} \end{cases} \quad (11.3)$$

so, for example, the quantity $\mathbf{F}\delta(t_i)$ is present only when $t_i = 0$. Similarly, the common phase ϕ is present only when $\xi_j = 0$, where ξ_j is a two value binary variable defined as:

$$\xi_j = \begin{cases} 1 & \text{If the } j\text{th sinusoid has a common zero order phase} \\ 0 & \text{Otherwise} \end{cases} . \quad (11.4)$$

Here common zero phase means that several sinusoids share the same zero order phase parameter.

The value of ξ_j is under user control. If the user selects the ‘‘Common’’ phase model, then $\xi_j = 0$ for all sinusoids and all sinusoids share the same common zero order phase parameter. If the user selects the ‘‘Independent’’ phase model, then $\xi_j = 1$ for all sinusoids and all sinusoids have a unique zero order phase parameter ϕ_j . Finally, if the user selects the phase model as ‘‘Independent’’ then the parameters ξ_j are binary variables that are simulated in the Markov chain Monte Carlo simulation, i.e., the Bayes Find Resonances package automatically determines which resonances have common zero order phase and which have a unique zero order phase.

Whether or not the constant models are present is also under user control. If the ‘‘Constant’’ check box is activated, then ν is set equal to zero by the package and $\delta(\nu) = 1$ and in Eq (11.2) the constant models are present. If the constant check box is not active then $\nu = 1$ and no constants are present in Eq (11.2). However, unlike the phase model, the Bayes Find Resonances package does not simulate the binary variable ν , this value is set by the user and the package uses the indicated value.

The Bayes Find Resonances package is a hybrid parameter estimation and model selection package. It is model selection in that it must determine how many resonances are present, and when the phase model is selected as ‘‘Independent’’ it must also estimate the binary parameters, ξ_j . So, the set of parameters estimated by Bayes Find Resonances package when all parameters are active, is:

F is the complex first point model, it contains two constants F_R and F_I , the real and imaginary first point parameters.

C is the complex constant offset model, it contains two constants C_R and C_I , which are the real and imaginary offset parameters.

m is the unknown number of sinusoids in the data.

A is the collection of amplitudes in the m sinusoids, so $A \equiv \{A_1, \dots, A_m\}$.

f is the collection of frequencies in the m sinusoids, so $f \equiv \{f_1, \dots, f_m\}$.

α is the collection of decay rate constants in the m sinusoids, so $\alpha \equiv \{\alpha_1, \dots, \alpha_m\}$.

t_0 is the first order phase in in the m sinusoids.

ξ is the collection of phase model indicators in the m sinusoids, so $\xi \equiv \{\xi_1, \dots, \xi_m\}$.

ϕ is the common zero order phase in the j th sinusoids when $\delta(\xi_j) = 1$.

ϕ_j is the zero order phase in the j th sinusoids when $\delta(\xi_j) = 0$.

We are going to designate this collection of parameters as Φ and then proceed with the Bayesian calculations.

The Bayesian calculations are for the posterior probability for the number of resonances in the data set. This posterior probability is designated as $P(m|DI)$, where D represents all of the data and I stands for all of the prior information. This posterior probability is computed by application of Bayes' Theorem:

$$P(m|DI) = \frac{P(m|I)P(D|mI)}{P(D|I)} \quad (11.5)$$

where $p(m|I)$ is the prior probability for the number of resonances, $P(D|mI)$ is the marginal direct probability for the data given the model order and $P(D|I)$ is a marginal direct probability for the data given only the prior information I . The direct probability for the data given only the prior information, $P(D|I)$, is a normalization constant and is given by:

$$\begin{aligned} P(D|I) &= \sum_{m=1}^{\text{Max}} P(Dm|I) \\ &= \sum_{m=1}^{\text{Max}} P(m|I)P(D|mI) \end{aligned} \quad (11.6)$$

where the maximum number of resonances is designated as "Max." Comparing, Eq. (11.6) to Eq. (11.5) it is easy to see that $P(D|I)$ is a normalization constant. If we normalize the posterior probability for the number of resonances, $P(m|DI)$, at the end of the calculations, then Eq (11.5) becomes:

$$P(m|DI) \propto P(m|I)P(D|mI). \quad (11.7)$$

The prior probability for the number of resonances, $P(m|I)$, is sufficiently simplified that we could assign it a numerical value. For now we will simply leave it in this symbolic form. However, the direct probability for the data given the number of resonances and the prior information, $P(D|mI)$, is not yet sufficiently simplified so that its value can be assigned. To proceed with the calculation, one introduces the collection of parameters Φ into this probability, the the direct probability for the data, $P(D|mI)$, the posterior probability for the number of resonances becomes

$$P(m|DI) \propto P(m|I) \int P(D\Phi|mI)d\Phi. \quad (11.8)$$

One proceeds by applying the product rule to the right-hand side of this equation:

$$P(m|DI) \propto P(m|I) \int P(\Phi|I)P(D|\Phi mI)d\Phi. \quad (11.9)$$

Factoring the prior probability for all of the parameters, $P(\Phi|I)$ into individual prior probabilities

for each parameter, one obtains:

$$\begin{aligned}
P(m|DI) &\propto P(m|I) \int P(F_R|I)P(F_I|I)P(C_R|I)P(C_I|I) \\
&\times P(\phi|I)P(t_0|I)P(D|\Phi mI) \\
&\times \left[\prod_{j=1}^m P(A_j|I) \right] \\
&\times \left[\prod_{j=1}^m P(f_j|I) \right] \\
&\times \left[\prod_{j=1}^m P(\alpha_j|I) \right] \\
&\times \left[\prod_{j=1}^m P(\xi_j|I) \right] \\
&\times \left[\prod_{j=1}^m P(\phi_j|I)^{\delta(\xi_j)} \right] d\Phi.
\end{aligned} \tag{11.10}$$

However, this is the marginal posterior probability for the number of resonances, and is the main output from the Bayes Find Resonances package. But the quantity sampled in the Markov chain Monte Carlo simulation is the joint posterior probability for all of the parameters. While this posterior probability is very similar, its not quite the same. The joint posterior probability for all of the parameters is given by:

$$\begin{aligned}
P(m\Phi|DI) &\propto P(m|I)P(F_R|I)P(F_I|I)P(C_R|I)P(C_I|I) \\
&\times P(\phi|I)P(t_0|I)P(D|\Phi mI) \\
&\times \left[\prod_{j=1}^m P(A_j|I) \right] \\
&\times \left[\prod_{j=1}^m P(f_j|I) \right] \\
&\times \left[\prod_{j=1}^m P(\alpha_j|I) \right] \\
&\times \left[\prod_{j=1}^m P(\xi_j|I) \right] \\
&\times \left[\prod_{j=1}^m P(\phi_j|I)^{\delta(\xi_j)} \right]
\end{aligned} \tag{11.11}$$

which is Eq. (11.10) without the integrations. The prior probabilities are assigned as follows:

$P(m|I)$ is assigned as an Exponential prior with $(0 \leq m \leq 50)$ where a model containing 50 resonances is a hard-coded maximum.

$P(F_R|I)$ is assigned as a bounded Gaussian prior whose range is $\pm 6 \times$ the amplitude of the first data value and whose standard deviation is three times the magnitude of the first data value.

$P(F_I|I)$ is assigned the same as $P(F_R|I)$ was assigned.

$P(C_R|I)$ is assigned as a bounded Gaussian whose mean is equal to the average of the last 10 real data values and whose upper and lower bounds is 5 times the mean. Finally, the standard deviation of this prior is one fifth of the prior range.

$P(C_I|I)$ is assigned like $P(C_R|I)$ except the means and bounds are taken from the imaginary channel.

$P(\phi|I)$ is assigned a uniform prior probability ranging from zero to 2π .

$P(t_0|I)$ essentially sets a time when the phases of all the sinusoids are the same. The prior probability for this time offset has a mean of zero, meaning that the phases are all expected to be the same at the start of the acquisition. However, we allow this parameter to range over ± 5 dwell or sampling times, i.e., the zero of time could occur the equivalent of 5 data values before the start of the acquisition and up to 5 data value past the start of acquisition. However, the standard deviation of this Gaussian prior probability is only 0.3 data values. Indicating, that while T_0 is allowed to have a large range, in fact it is strongly suspected that its value is near zero.

$P(A_j|I)$ is assigned a bounded Gaussian prior probability for one of the amplitudes. Its mean is zero, its upper and lower bounds are 3 times the average magnitude of the first 10 complex data values and its standard deviation is two times that average. This prior is used for the prior probability for each resonance amplitude in the model.

$P(f_j|I)$ is assigned a uniform prior probability ranging over the entire sweep width of the data. This prior is used for the prior probability for each resonance frequency in the model.

$P(\alpha_j|I)$ is assigned a positive prior probability whose low is 0.001 in dimensionless units. The peak value is set to the current value of the “lb” parameter. The maximum value is set so that if the signal were decaying at this maximum, it will go through roughly 3 e-foldings in the first 9 data values. So the maximum value is strongly dependent on the sampling rate.

$P(\xi_j|I)$ is assigned a discrete uniform prior probability having two possible values, zero or one with zero indicating an independent phase and one indicating a common phase.

$P(\phi_j|I)$ is assigned a uniform prior probability ranging from zero to 2π . In the above equations, [11.10](#) and [11.11](#), this probability is written as $P(\phi_j|I)^{\delta(\xi_j)}$, which is just a notational mechanism to indicate that the prior is either present or not. When $\delta(\xi_j) = 1$, $\xi_j = 0$, the phase model is independent and the prior is present. Similarly, when $\xi_j = 1$ the phase model is common and this prior is not present because the prior is raised to the zero power.

$P(D|\Phi m I)$ is the direct probability for the data given all of the parameters and the prior information and is assigned using a Gaussian prior probability for the noise. This probability is often called a likelihood or likelihood function.

The Markov chain simulation that implements this calculation targets the joint posterior probability for all of the parameters in the model, Eq. [\(11.11\)](#). It then uses Monte Carlo integration to obtain samples from the marginal posterior probability for each parameter appearing in the model. The samples from the marginal posterior probability for each parameter are then used to generate mean and standard deviation estimates of each parameter appearing in the model. Additionally, the samples are used to generate histograms. These histograms are crude estimates of the posterior probability for each parameter. In addition to outputting the histograms, the samples are also output and these samples can be used to generate Maximum Entropy histograms of the samples, see

Section (??). Finally, these samples are used to compute the posterior probability for the number of resonances, Eq. (11.10).

If there are multiple high probability models in this posterior, i.e., the posterior probability for the number of resonances, $P(m|DI)$, has significant weight on several values of m , then samples are drawn for each high probability model and these samples are used to generate histograms and parameter estimates given each high probability model. Consequently, then the algorithm finishes it is possible to have not one set of outputs but several. These outputs are viewed using the standard widgets. Additionally, it is possible to generate time domain FID models for each high probability model.

11.2 Outputs From The Bayes Find Resonances Package

The Text outputs files from the Find Resonance packages consist of: “Bayes.prob.model,” “BayesFind-Res.mcmc.values,” “Bayes.params,” “Console.log,” “Bayes.accepted” and a “Bayes.Condensed.File.” These output files can be viewed using the Text Viewer or they can be viewed using File Viewer by navigating to the current working directory and then selecting the files. The format of the mcmc.values report is discussed in Appendix D and the other reports are discussed in Chapter 3. Additionally, the “Plot Results Viewer” can be used to view the output probability density functions. In addition to the standard data, model and residual plots there are probability density functions for the frequencies and decay rate constants, and the amplitudes for each resonance for each high probability model.

Finally, for each high probability model, there is an output “bayes.params.nnnn” and “bayes.model.nnnn” file where this file has exactly the same format as the Bayes Analyze Model file, see Chapter 8.5.7. These files are used in conjunction with the “Build FID Model” button to generate a time domain model of the input FID data. When this button is activated the FID and the selected bayes.model.nnnn file are sent to the server and the Bayes Model program, see Chapter 8.1 for a description of this program, is run. During this time the interface waits for the Bayes Model program to finish. When the interface detects that the model has been built, the interface fetches the model from the server, Fourier transforms the model and then displays the model using the FID Model Viewer.

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.