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

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Chapter 5

Given Exponential Model

The Given Exponential Package estimates amplitudes and decay rate constants in data that are known to contain signals which are sums of exponentials. This signal may or may not contain a constant offset, and the number of exponentials in the data need not be known. The calculations presented in this Chapter describe the given model, i.e., given the number of exponentials and whether a constant is or is not present. We describe the calculations for the unknown number of exponentials in Chapter 6. The input data files analyzed by this package are Ascii and may be input from Ascii files, a peak pick, a Bayes Analyze file or they may be loaded from an image pixel. When "Exponential" package button is activated, the interface window shown in Fig. 5.1 is displayed. This is the interface for both "Given" and "Unknown" number of exponentials. To use this package, you must do the following:

Select the exponential package from the Package menu.

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.

Set the number of exponentials in the model using the Model/Order selection menu.

Check the Model/Constant box if the data contains an offset.

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

Review the prior probabilities for the decay rate constant using the Prior Viewer.

Select the server that is to process the analysis.

Check the status of the selected server to determine if the server is busy, change to another server if the selected server is busy.

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

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.

Figure 5.1: The Given And Unknown Number Of Exponential Package Interface

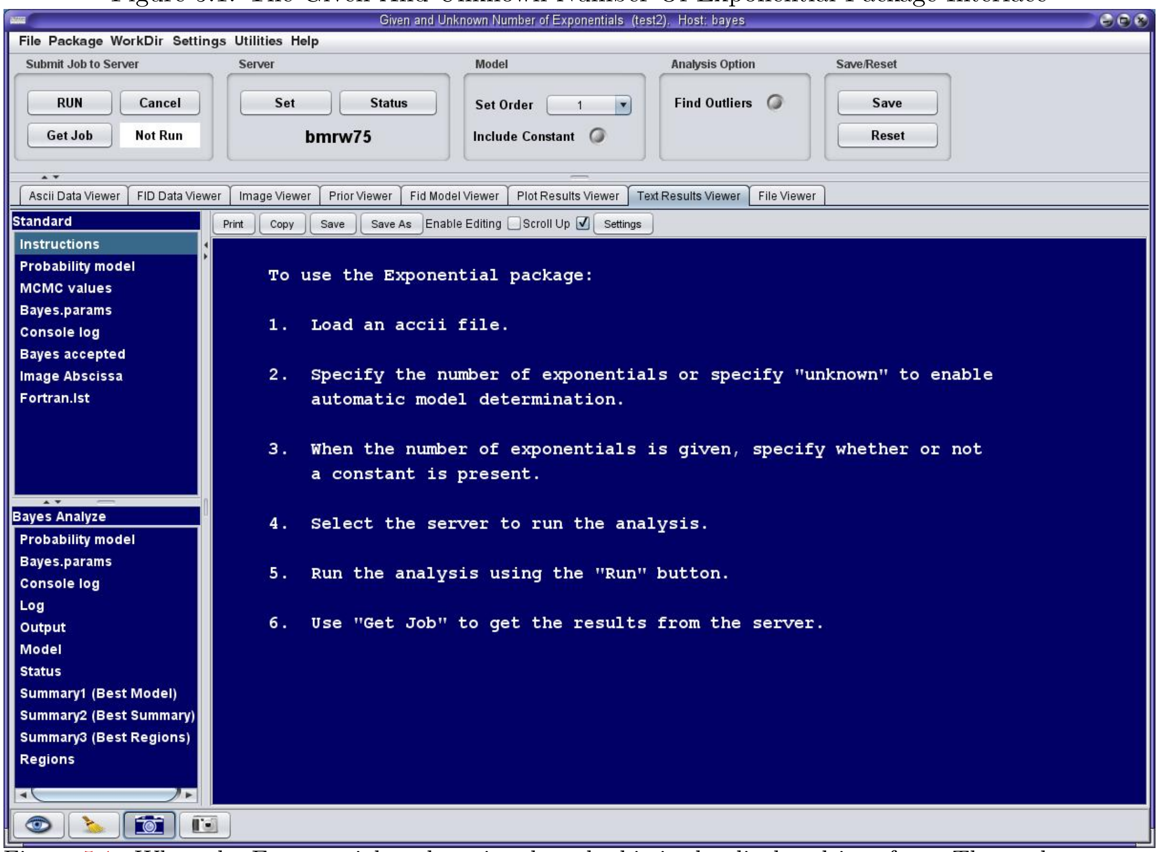

Figure 5.1: When the Exponential package is selected, this is the displayed interface. The package setup widgets, in this case labeled "Model," allow you to select the number of exponentials in the data and they allow you to specify whether or not a constant offset is present. Additionally, the prior viewer can be used to set the prior probability for the decay rate constants. Note in this package the posterior probabilities are marginal posterior probabilities, so there are no adjustable prior probabilities for the amplitudes.

5.1 The Bayesian Calculation

The sums of exponential package process data that are known to contain exponential signals of the form:

$$d_{ik} = C_k + \sum_{j=1}^{m} A_{jk} \exp\{-\alpha_j t_{ik}\} + n_{ik} \tag{5.1}$$

where d_{ik} is the ith data value in the kth data set, C_k is the constant offset in the kth data set, m is the number of exponentials, A_{jk} is the amplitude or intensity of the jth exponential in the kth data set, α_j is the jth exponential decay rate constant, t_{ik} is the ith abscissa value in the kth data set, and as this equation implies, the abscissa values and the sampling times need not be the same from one data set to the next. In Fig. 5.1, the model widgets, allow you to set the number of exponentials and allow you to indicate if a constant is present. Additionally, the prior viewer can be used to set the prior probability for the decay rate constants. Finally, the number of data sets n is determined by the number of Ascii data sets loaded into the analysis. If 5 Ascii data sets are loaded, the $n = 5$.

When the number of exponentials are given, the problem is one of parameter estimation and the program that implements this Bayesian calculation computes the marginal posterior probability for each of the parameters appearing in the model. For example, the marginal posterior probability for the decay rate constant, α_j, is computed from the joint posterior probability for all of the parameters using the sum rule:

$$P(\alpha_j|DI) = \int d\{A\}d\{C\}d\{\sigma\}d\alpha_1 \ldots d\alpha_{j-1}d\alpha_{j+1} \ldots d\alpha_m P(\{A\}\{C\}\{\sigma\}\{\alpha\}|DI) \tag{5.2}$$

where the integral is over all of the parameters except the parameter of interest, in this case α_j. The notation, $\{\cdot\}$ is being used to stand for all of the enclosed quantities. So for example if there are three exponentials and 5 data sets, there are 15 total amplitudes represented by $\{A\}$. Similarly, because there is one constant per data set, then there would be 5 total constants represented by $\{C\}$. The right-hand side of this equation was factored using the rules of probability theory and Bayes Theorems' [1]

$$\begin{aligned} P(\{A\}\{C\}\{\sigma\}\{\alpha\}|DI) \quad &\propto \quad \left[\prod_{l=1}^{m} P(\alpha_l|I)\right] \\ &\times \quad \left[\prod_{k=1}^{n} P(C_k|I)P(\sigma_k|I)\right] \\ &\times \quad \left[\prod_{k=1}^{n}\prod_{j=1}^{m} P(A_{jk}|I)\right] \\ &\times \quad \left[\prod_{k=1}^{n} P(D_k|\{A\}_k\{\alpha\}C_k\sigma_k I)\right] \end{aligned} \tag{5.3}$$

where m is the given number of exponentials, n is the number of data sets, $P(\alpha_l|I)$ is the prior probability for the lth decay rate constants, $P(C_k|I)$ is the prior probability for the constant in the kth data set, $P(\sigma_k|I)$ is the prior probability for the standard deviation of the noise, $P(A_{jk}|I)$ is the prior probability for the amplitudes of the jth exponential in the kth data set, and $P(D_k|\{A\}_k\{\alpha\}C_k\sigma_k I)$

is the direct probability or likelihood of data set D_k given the amplitudes, $\{A\}_k$, in the kth data set, the constant offset, C_k, and the standard deviation of the noise, σ_k.

The various probabilities are assigned as follows The prior probability for the decay rate constant, $P(\alpha_l|I)$ are user defined and the functional form of this prior probability can be any of the following: a uniform prior probability, a bounded Gaussian, an exponential prior probability or a prior positive. When the interface initializes the exponential package, a default prior probability for the decay rate constant is defined using the maximum value of the abscissa. This default prior probability is a bounded Gaussian prior probability that goes through 4.5 e-foldings over the decay rate constant ranges shown in the interface. If the maximum decay rate constant is α_{Max}, then the default prior probability for the decay rate constant is given by

$$P(\alpha_l|I) = \begin{cases} \frac{1}{N_l}\exp\{-\frac{\alpha_l^2}{2\sigma_l^2}\} & \text{if } (0 \le \alpha_l \le \alpha_{\text{Max}}) \\ 0 & \text{otherwise} \end{cases} \tag{5.4}$$

where N_l is a normalization constant. If we make the assumption that the exponential signal components decay to no more than 20 e-foldings over the run of the data, then we can define a maximum decay rate constant:

$$\alpha_{\text{Max}} T_{\text{Max}} \equiv 20, \tag{5.5}$$

T_{Max} is the maximum abscissa value, so

$$\alpha_{\text{Max}} = \frac{20}{T_{\text{Max}}}, \tag{5.6}$$

and σ_l is set so that the prior goes through 4.5 e-foldings:

$$\frac{(\alpha_{\text{Max}})^2}{2\sigma_l^2} = 4.5. \tag{5.7}$$

Consequently,

$$\sigma_l \approx \frac{6.666666}{T_{\text{Max}}}. \tag{5.8}$$

The user assigns only a single prior probability for the decay rate constants and the interface uses this prior for all decay rate constants.

The prior probabilities for the amplitudes, the $P(A_{jk}|I)$, are assigned using broad Gaussian that range from $-\infty$ to $+\infty$,

$$P(A_{jk}|I) = \left(\frac{2\pi\sigma_k^2}{\delta^2}\right)^{-\frac{1}{2}} \exp\left\{-\frac{\delta^2}{2\sigma_k^2}A_{jk}^2\right\} \tag{5.9}$$

where $\delta = 0.01$ in the given and unknown number of exponentials. In these package you cannot change the prior probability for the amplitudes. Similarly, the prior probability for the constant offset in each data set, $P(C_k|I)$, is also assigned as a Gaussian prior probability using

$$P(C_k|I) = \left(\frac{2\pi\sigma_k^2}{\delta^2}\right)^{-\frac{1}{2}} \exp\left\{-\frac{\delta^2}{2\sigma_k^2}C_k^2\right\} \tag{5.10}$$

the same functional form with δ also equal to 0.01. Consequently, it is possible for this package to estimate either the amplitudes or the constant offsets to be negative when the prior information available to the user would constrain it to be positive. If this is unacceptable, in the Enter Ascii Model package there is a full suite of exponential models that allow you to control the prior range on the amplitudes as well as the decay rate constants, Chapter 20. The prior probability for the standard deviation of the noise, the σ_k, were assigned using Jeffreys' priors [33],

$$P(\sigma_k|I) \propto \frac{1}{\sigma_k}. \tag{5.11}$$

Finally, the direct probability for the data was assigned using a Gaussian likelihood function. This Gaussian had a standard deviation given by σ_k that is specific to each data set.

The exponential model equation, Eq. (5.1) is symmetric under relabeling of the amplitudes and decay rate constants. This symmetry causes the joint posterior probability for the decay rate constants to be symmetric in the sense that if there is a peak at $\alpha_1 = \beta$ and $\alpha_2 = \gamma$, then there is also a peak at $\alpha_1 = \gamma$ and $\alpha_2 = \beta$; this symmetry is caused because the model does not tell us which exponential signal corresponds to to which model component. Consequently, a convention must be introduced which brakes this symmetry. In the calculations implemented here, we break this symmetry by ordering the rate constants: $\{\alpha_1 < \alpha_2 < \alpha_3, \mathrm{etc.}\}$.

The full Bayesian calculation and the assignment of the prior probabilities is discussed in reference [15] and this paper is available in pdf by activating this link. Additionally, much more about exponential parameter estimation is contained in [16, 17]. The first paper describes the problem of determining the number of exponentials in a given sample of data, while the second paper discusses how the accuracy of the parameter estimates depends on the number of data values, signal-to-noise level and the rate of decay of the sample.

5.2 Outputs From The Given Exponential Package

The Text outputs files from the exponential packages consist of: "Bayes.prob.model," "BayesExpGiven.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 decay rate constants, decay times, the amplitudes for each data set for each exponential and finally there are probability density functions for the standard deviation of the noise in each data set.

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