Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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Chapter 16

Given Polynomial Order

The Given polynomial Order package fits polynomials to two column Ascii data when the order of the polynomial is known. The interface to the Given Polynomial Order package is shown in Figure16.1. This interface differs from most others in one respect, there are no parameter ranges to enter, so use of the interface is particularly simple. To use this package, you must do the following:

Select the Polynomial Models package from the Package menu. When selected this menu will bring up the "Given" and "Unknown" polynomial model interface.

Load one two column Ascii data sets. The data may be loaded using the Files menu. You can also load an arrayed Fid and then use a single cursor to mark the center of a peak and use the "Get Peak" button on the bottom right of the Fid viewer. Finally, the "Files/Load Ascii/Bayes Analyze" button can be used to load an Ascii data set from the amplitudes estimated by Bayes Analyze. When a data set is successfully loaded the data is plotted in the Ascii Data viewer. This package does not allow you to run with multiple data sets. If you attempt to do so, you will be prompted to remove all but a single file.

Set the Polynomial order using the "Set Order" selection widget. For the Given Polynomial Order, the order can be from 1 to 55.

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 16.1: Given Polynomial Order Package Interface

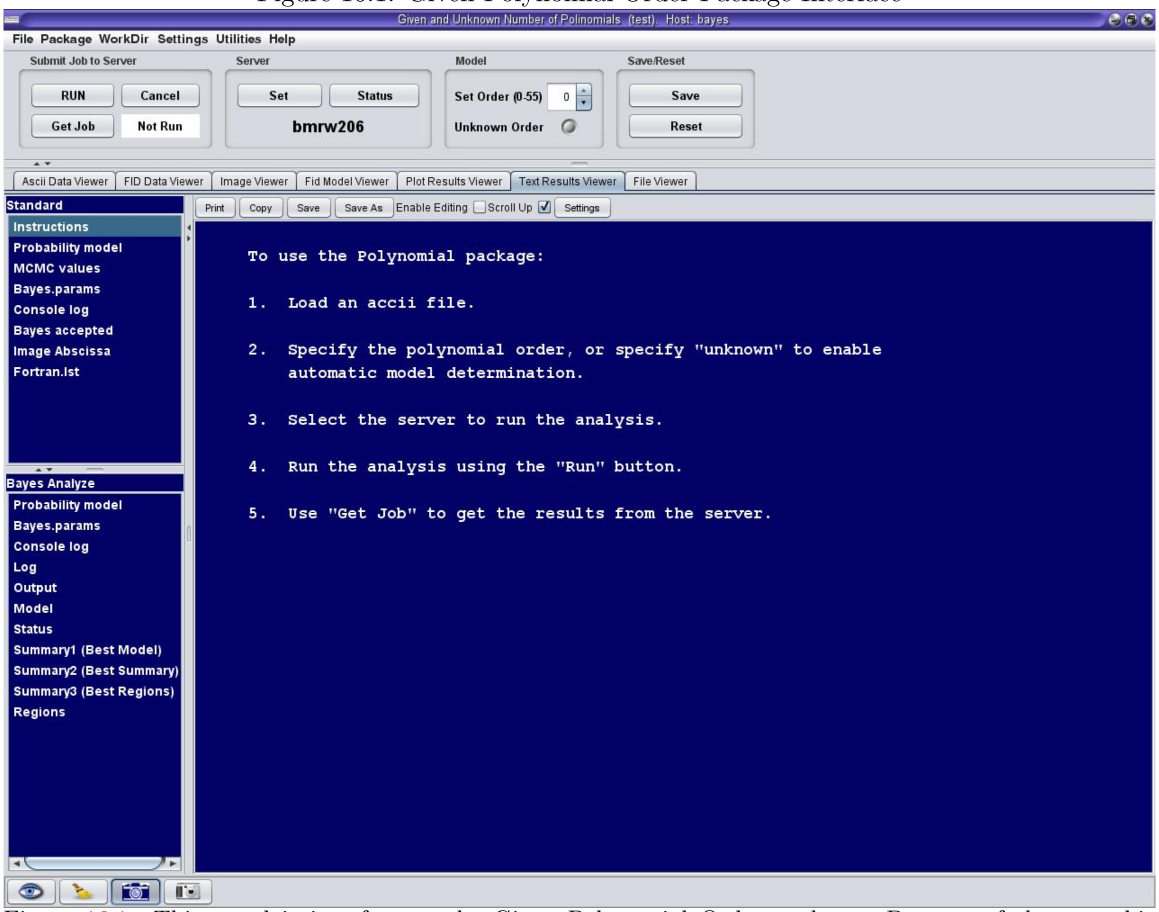

Figure 16.1: This panel is interface to the Given Polynomial Order package. Because of the way this calculation is done very high orders are possible and numerically stable. However, the high orders, above 40, require very high signal-to-noise and even then roundoff errors degrade the accuracy to 4 or 5 decimal places.

16.1 The Bayesian Calculation

The polynomial model is just that, its a model in which a polynomial is fit to the data:

$$d_i = \sum_{j=0}^{m} A_j G_j(t_i) + n_i \tag{16.1}$$

with

$$G_j(t_i) = t_i^j \tag{16.2}$$

where A_j is the amplitude of the jth polynomial, n_i represents noise in the ith data value and we have written these polynomials as $G_j(t_i)$ for notational convenience. We will think of these polynomials as functions of time, but in the analysis which follows t is simply a single column abscissa and may be any quantity. In the problem we are describing here, m is the given order of the polynomial. Additionally, the assumption that these are polynomials is unimportant in the following discussions, the $G_j(t_i)$ could be any set of functions.

16.1.1 Gram-Schmidt

The Bayesian calculation is implemented using Markov chain Monte Carlo with simulated annealing to draw samples for the joint posterior probability for the parameters. Before we do this calculation we introduce a change of function and a change of variables. The reason for this is simply that computing polynomials of the form $\sum_{j=0}^{m} A_j t_i^j$ is computationally vary unstable in the sense that only orders up to about 8 can be computed using single precision arithmetic. You can get to higher orders only by using numerical procedures that avoid differencing large numbers, for example the remainder theorem. However, here we take a different approach by transforming the problem to something that is computationally more stable. Using Gram-Schmidt, the polynomials are transformed to a set of orthogonal polynomials. We then solve the problem using these orthogonal polynomials and finally, we transform the derived amplitudes back to the A_j given in Eq. (16.1). If we designate the Gram-Schmidt polynomials as $H_j(t_i)$ and the expansion coefficients as B_j, Eq. (16.1) becomes:

$$d_i = \sum_{j=0}^{m} B_j H_j(t_i) + n_i. \tag{16.3}$$

We chose the Gram-Schmidt polynomials because they can be computed trivially from the t_i^j, they preserve the notation of the order of the polynomial, and each polynomial depends only on the lower orders, not the higher orders. This change of variables and change of function is an identity, i.e., the polynomial expansions in Eq. (16.1) and Eq. (16.3) are exactly equal to each other. Finally, the amplitudes, B_j and A_j, are linearly related to each other through an lower triangular matrix, and consequently, the conversion back and forth between these representations is very easy to program.

As a reminder to those unfamiliar with Gram-Schmidt polynomials, the normalized Gram-Schmidt polynomials $H_j(t_i)$, are generated recursively from the $G_j(t_i)$ using:

$$H_j(t_i) = \frac{1}{C_{jj}} \left[G_j(t_i) - \sum_{\ell=0}^{j-1} C_{j\ell} H_\ell(t_i) \right] \tag{16.4}$$

where the sum is not present for the first polynomial, and

$$C_{j\ell} = \sum_{i=1}^{N} G_j(t_i) H_\ell(t_i) \qquad (0 \leq j \leq \ell). \tag{16.5}$$

Gram-Schmidt polynomials have the property

$$\sum_{i=1}^{N} H_j(t_i) H_\ell(t_i) = \delta_{j\ell} \tag{16.6}$$

where $\delta_{j\ell}$ is zero if $j \neq \ell$ and one if $j = \ell$.

To derive the relationship between the A_j and the B_j, note that the expansions given by Eq. (16.1) and Eq. (16.3) are identities, so can write

$$\sum_{k=0}^{m} A_k G_k(t_i) = \sum_{j=0}^{m} B_j H_j(t_i) \tag{16.7}$$

where we changed the summation index on the left-hand side just to remind people that these summations are independent of each other. Multiplying this equation by $H_\ell(t_i)$, and summing over time:

$$\sum_{i=1}^{N} \sum_{k=0}^{m} A_k G_k(t_i) H_\ell(t_i) = \sum_{i=1}^{N} \sum_{j=0}^{m} B_j H_j(t_i) H_\ell(t_i). \tag{16.8}$$

The right-hand side of this equating is zero unless $j = \ell$ and then one obtains

$$\sum_{i=1}^{N} \sum_{k=0}^{m} A_k G_k(t_i) H_\ell(t_i) = B_j \tag{16.9}$$

and the sum over time on the left-hand side of this equation can be written as

$$\sum_{k=0}^{m} A_k \left[\sum_{i=1}^{N} G_k(t_i) H_\ell(t_i) \right] = B_j. \tag{16.10}$$

The quantity in big square brackets is just the right-hand side of Eq. (16.5), so this equation becomes

$$\sum_{k=0}^{m} A_k C_{k\ell} = B_\ell. \tag{16.11}$$

The matrix $C_{k\ell}$ is a lower triangular matrix, so inverting it is trivial and one can use this equation solve for the nonorthogonal expansion coefficients, the A_k, from the orthogonal expansion coefficients, the B_j.

16.1.2 The Bayesian Calculation

The Bayesian calculation is for the joint posterior probability for the amplitudes, B_j, given the data and the prior information. This joint probability, denoted by $P(B_0 B_1 \ldots B_m|DI)$, is computed by application of Bayes' theorem

$$P(B_0 B_1 \ldots B_m|DI) \propto P(B_0 B_1 \ldots B_m|I) P(D|B_0 B_1 \ldots B_m I) \tag{16.12}$$

where $P(B_0 B_1 \ldots B_m|I)$ is the joint prior probability for the amplitudes, and $P(D|B_0 B_1 \ldots B_m I)$ is the likelihood. Because each polynomial is orthogonal, we will factor the joint prior probability for the amplitudes, $P(B_0 B_1 \ldots B_m|I)$, into a series of independent prior probabilities:

$$P(B_0 B_1 \ldots B_m|I) = \prod_{j=0}^{m} P(B_j|I) \tag{16.13}$$

and each of the $P(B_j|I)$ will be assigned a unbound Gaussian. The posterior probability for the B_j, is thus given by:

$$P(B_0 B_1 \ldots B_m|DI) \propto \left[\prod_{j=0}^{m} P(B_j|I)\right] P(D|B_0 B_1 \ldots B_m I). \tag{16.14}$$

We want the Markov chain to explore the amplitude parameter space, but we don't want it to excessively waist time. All the amplitudes in an orthogonal model are estimated to be $\pm\sqrt{\langle\sigma^2\rangle}$, where $\langle\sigma^2\rangle$ is the mean-square residual given the model. Consequently, if we center the prior probability for an amplitude on the expected amplitude, T_j Eq. (16.16) below, and make the standard deviation of the prior very wide, then the prior probability for the amplitudes will do little more than keep the Markov chain in the physically meaningful region of the parameter space. Here is the prior actually used for the amplitudes:

$$P(B_j|I) = \left(2\pi\delta^2\right)^{-\frac{1}{2}} \exp\left\{-\frac{(T_j - B_j)^2}{2\delta^2}\right\} \tag{16.15}$$

where the expected amplitude, T_j, is given by

$$T_j \equiv \sum_{i=1}^{N} d_i H_j(t_i) \tag{16.16}$$

where N is the total number of data values in the data set. The standard deviation of this prior, δ, is 10 times larger than the expected root mean-square residual:

$$\delta = 10\sqrt{\langle\sigma^2\rangle} \tag{16.17}$$

with

$$\sqrt{\langle\sigma^2\rangle} = \sqrt{\frac{\overline{d^2} - \overline{h^2}}{N}}. \tag{16.18}$$

The quantity, $\overline{d^2} - \overline{h^2}$, is the total-squared residual given the polynomial. So the square root is the root mean-square residual given the polynomial order. The sufficient statistic, $\overline{h^2}$, is the total-squared projection of the data onto the polynomial and is defined as

$$\overline{h^2} \equiv \sum_{k=0}^{m} T_k^2. \tag{16.19}$$

Having assigned the prior probabilities, we must now assign the direct probability. The direct probability, $P(D|B_0 B_1 \ldots B_m I)$, is a marginal probability and is computed from the joint probability for the data and the standard deviation of the noise

$$P(D|B_0 B_1 \ldots B_m I) = \int P(\sigma D|B_0 B_1 \ldots B_m I) d\sigma \tag{16.20}$$

which we factor as

$$P(D|B_0B_1\dots B_mI) = \int P(\sigma|I)P(D|\sigma B_0B_1\dots B_mI)d\sigma. \tag{16.21}$$

Assigning a Jeffreys' prior to $P(\sigma|I)$ and a Gaussian likelihood, one obtains

$$P(B_0B_1\dots B_m|DI) \propto \left[\prod_{j=0}^{m} P(B_j|I)\right] \int \frac{1}{\sigma}\left(2\pi\sigma^2\right)^{-\frac{N}{2}} \exp\left\{-\frac{Q}{2\sigma^2}\right\} d\sigma \tag{16.22}$$

where we have left the prior probabilities in their symbolic form. Evaluating the integral over σ and substituting the prior probability for the amplitudes, Eq. (16.15), into Eq. (16.22), one obtains:

$$P(B_0B_1\dots B_m|DI) \propto \left[\prod_{j=0}^{m} \exp\left\{-\frac{(T_j - B_j)^2}{2\delta^2}\right\}\right] \left[\frac{Q}{2}\right]^{-\frac{N}{2}} \tag{16.23}$$

where we dropped some constant terms that cancel when this probability is normalized. The function Q is defined as

$$\begin{aligned} Q &\equiv \sum_{i=1}^{N}\left(d_i - \sum_{j=0}^{m} B_j H_j(t_i)\right)^2 \\ &= N\overline{d^2} - 2\sum_{j=0}^{m} B_j T_j + \sum_{j=0}^{m} B_j^2. \end{aligned} \tag{16.24}$$

One interesting note about the quantity Q, it does not depend on the individual data values, rather it depends on the total squared data value, the $N\overline{d^2}$, and it depends on the projection of the data onto the orthogonal functions, the T_j. Both of these items can be computed at the beginning of the calculation and used throughout with no further reference to the data. Consequently, the Given Polynomial Order runs very quickly. Also, note that the function Q could have been written as a single summation rather than two. If the standard deviation for the noise is known, the posterior probability for the B_j can be factored into a product of probabilities for each amplitude separately, i.e., the amplitudes of the orthogonal polynomials may be estimated separately, they don't have to be estimated jointly. Finally, because each amplitude can be estimated separately, one can simply plot the posterior probability for each amplitude, there is no need to use a Markov chain Monte Carlo simulation to sample the joint posterior. However, joint estimation is required after marginalizing out the standard deviation for the noise. The joint estimation is done using a Markov chain Monte Carlo simulation to sample the joint posterior probability for the amplitudes, Eq. (16.23).

16.2 Outputs From the Given Polynomial Order Package

The Text outputs files from the Given Polynomial Order package consist of: "Bayes.prob.model," "BayesPolGiven.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

Figure 16.2: Given Polynomial Order Scatter Plot

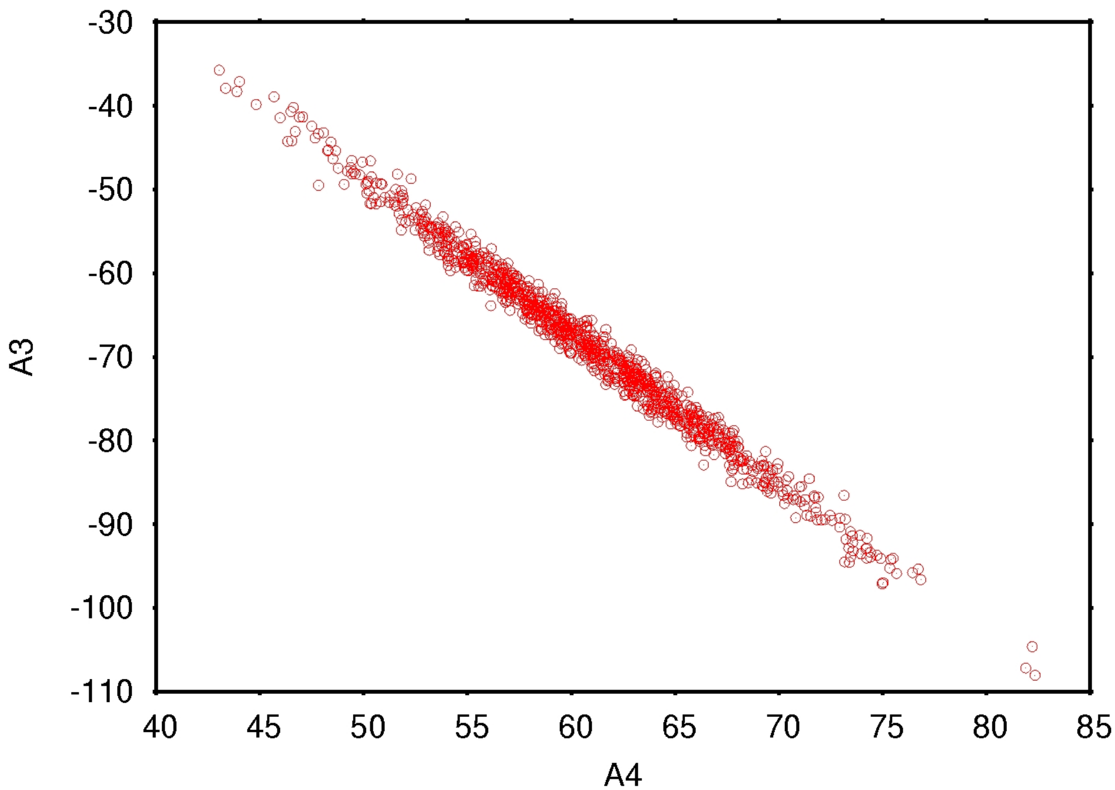

Figure 16.2 The expansion coefficients in a nonorthogonal polynomial expansion tend to be highly correlated. Plotted here is a scatter plot of the 3rd and 4th order expansion coefficients, A_3 and A_4, as generated by a 6th order expansion of the 6th order polynomial test data. This test data can be downloaded using the "Files" menu.

mcmc.values report is discussed in Appendix D and the other reports are discussed in Chapter 3. Additionally, the "Plot Results Viewer" can be used to view the output probability density functions. In addition to the standard data, model and residual plots there are probability density functions for each A_j in the given model. And because estimation of the amplitudes in polynomial models tend to be highly correlated, there are covariance plots to help illustrate these correlations. These covariance plots are scatter plots. The scatter plots are generated from the samples drawn from the Markov chain Monte Carlo simulation. In a typical run, there might be 50 simulations and 30 repeats giving a total of 1500 simulations. Each of these simulations contain the estimated parameters from one Markov chain Monte Carlo simulation. A typical scatter plot just put a dot in the plot at the location of parameter 1 verses parameter 2. In this package that would correspond to plotting A_j verses A_k. In Fig. 16.2, A_3 verses A_4 is plotted. The data used to generate this figure are the 6th order polynomial expansion data available in our test data kit. This test data can be downloaded using the "Files" menu. The covariance plot shown in Fig. 16.2 is the one generated form the A_3 and A_4 expansion coefficients in a 6th order expansion of this data. For these two parameters there is a strong correlation, when A_3 increases the A_4 parameter decreases to counter the effect of changing A_3. Uncorrelated parameters, by contrast, will have elliptical scatter plots with the major and minor axis aligned with coordinate system. The number of possible scatter plots is $m(m+1)$ where m is the order of the polynomial. Because the number of scatter plots can become large very quickly, the package only outputs a representative sample of these plots.

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