Bayesian Inversion with TimeOptMCMC

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Abstract

TimeOptMCMC (Meyers and Malinverno, 2018) is a Bayesian approach for evaluating cyclostratigraphic records that quantitatively links geologic data with astronomical theory. This manuscript provides an introductory guide for conducting a TimeOptMCMC Bayesian inversion, following the approach of Meyers and Malinverno (2018). The purpose of this guide is to help users identify an appropriate data set for analysis, setup an inversion correctly, execute the inversion, post-process and interpret the results, and finally, provide appropriate documentation of the TimeOptMCMC inversion in their publication. An appendix includes numerous new scripts for executing the inversion and post-processing the MCMC results.

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Introduction

TimeOptMCMC (Meyers and Malinverno, 2018) is a Bayesian approach for evaluating cyclostratigraphic records that quantitatively links geologic data with astronomical theory. This manuscript provides an introductory guide for conducting a TimeOptMCMC Bayesian inversion, following the approach of Meyers and Malinverno (2018). The purpose of this guide is to help users identify an appropriate data set for analysis (**Part 1**), setup an inversion correctly (**Part 2**), execute the inversion (**Part 3**), post-process and interpret the results (**Part 4**), and finally, provide appropriate documentation of the TimeOptMCMC inversion in their publication (**Part 5**). The **Appendix** includes numerous new scripts for executing the inversion and post-processing the MCMC results.

This guide utilizes numerous functions in the 'astrochron' package for R (Meyers, 2014; https://cran.r-project.org/web/packages/astrochron/index.html), including 'timeOptMCMC', which executes the Bayesian inversion. The term 'TimeOptMCMC' refers to the statistical methodology, while 'timeOptMCMC' refers to the specific function in the astrochron package. Use of timeOptMCMC requires the installation of the software R (https://cran.r-project.org). The present document only considers the evaluation of eccentricity and precession signals in stratigraphic data, as in the original TimeOptMCMC methodology (Meyers and Malinverno, 2018). Improvements to the algorithm are ongoing (Malinverno and Meyers, 2024), such as inclusion of the evaluation of obliquity, updated priors, etc.; these updates will be addressed in a future guide.

> *NOTE 1: This tutorial assumes some general knowledge of Bayesian analysis and the Metropolis-Hastings approach. There are many details that are only briefly mentioned here, and we refer interested readers to more detailed discussions in Meyers and Malinverno (2018), and the references therein.*

> *NOTE 2: In the process of conducting the Bayesian MCMC analyses on your cyclostratigraphic dataset, you will also be exploring the algorithm. Each analysis of a data set potentially provides new insight into the computational approach, its effective execution on your dataset, and hopefully, new constraints on the astronomical cycles, fundamental frequencies, and Earth-Moon history.*

> *NOTE 3: Depending upon the specifics of a given cyclostratigraphic dataset – and assuming it is appropriate for TimeOptMCMC – the time required for a complete assessment and inversion(s) may range from a week to a month. This includes numerous test analyses to assure that the inversion is producing reliable results. As such, it is worthwhile to have a dedicated computer or virtual server to conduct the analysis, with uninterrupted power.*

Part 1: Identifying an appropriate data set for TimeOptMCMC analysis

The TimeOptMCMC approach requires high-quality cyclostratigraphic data to produce meaningful and reliable results. "What constitutes a high-quality data set?", you may ask. In order to determine if your stratigraphic series is appropriate for TimeOptMCMC, it is important to perform some initial analyses with the non-Bayesian formulation of TimeOpt (Meyers, 2015), to determine (1) if substantial power is present in the hypothesized climatic precession and eccentricity bands, and (2) if significant[1] results are obtained using plausible astronomical parameters and sedimentation rates. **If either of these cases is not satisfied, then the data set is *likely* not appropriate for TimeOptMCMC.**

The versions of TimeOpt and TimeOptMCMC implemented in this guide assume a constant sedimentation rate in the stratigraphic interval evaluated. Therefore, prior to evaluation with TimeOpt and TimeOptMCMC, it is also advisable to use time-frequency analysis (such as evolutive harmonic analysis, astrochron function 'eha'; Meyers et al., 2001) to identify stratigraphic intervals with relatively stable sedimentation. You may also consider using the evolutive version of TimeOpt (function 'eTimeOpt'). Versions of TimeOpt that allow for more complex sedimentation models (function 'timeOptTemplate', Meyers, 2019) exist, but this feature is still in development for TimeOptMCMC.

Note that your stratigraphic data set must be evenly sampled (have a consistent sample spacing), with a Nyquist frequency and stratigraphic length suitable for evaluating the astronomical terms of interest. This requires some knowledge of plausible sedimentation rates. Also note that, while detrending is a relatively common practice in cyclostratigraphy, it should be done with great caution, and is best avoided (beyond a simple linear detrending, which is generally a good idea). Finally, it is important to assemble all the supporting geochronologic and chronostratigraphic data (biostratigraphy, radioisotopic data, magnetostratigraphy, chemostratigraphy), as well as depositional basin constraints, sedimentologic/stratigraphic constraints, and paleoceanographic constraints that exist, to support your analyses and cyclostratigraphic interpretations. This information will also be critical in **Part 2**, for setting up the TimeOptMCMC Bayesian priors.

Relevant functions in 'astrochron', for the preliminary cyclostratigraphic assessment:

    read – read your data set
    linterp – interpolate your data series to an evenly sampled grid
    eha – evolutive harmonic analysis, a time-frequency approach
    iso – isolate portions of your dataset for analysis
    timeOpt – "Timescale Optimization" method for astronomical calibration and testing (Meyers, 2015)

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[1] Evaluating statistical significance is tricky business. It involves testing against a null model, but the appropriate null model is not always obvious. Furthermore, many of the commonly used methods for significance testing suffer from being too optimistic, while more 'rigorous' approaches are commonly overly pessimistic. A holistic approach is advocated here, which leverages correct use and reporting of statistical metrics, while also considering basin framework, paleoceanography, and additional supporting evidence in making inferences. See Meyers (2019) for a discussion.

periodogram – examine the background fit to your cyclostratigraphic data set, and look at some preliminary assessments of the statistical significance of power spectrum peaks (also see astrochron functions '**mtm**', '**mtmPL**')

timeOptSim – TimeOpt significance testing using Monte Carlo simulation with an AR1 stochastic null model

timeOptSimPwrLaw – TimeOpt significance testing using Monte Carlo simulation with a power law stochastic null model

Essential parameters for your initial TimeOpt analyses include the astronomical target periods, and the range of plausible (average, constant) sedimentation rates for the study interval. You can find potential astronomical parameters for your data set using David Waltham's 'Milankovitch Calculator' (Waltham, 2015), and in the recent work of Farhat et al. (2022) and Hoang et al. (2021). There are also a range of functions built into 'astrochron', such as 'etp', 'bergerPeriods', 'calcPeriods', that can be used for this purpose. Estimates of plausible sedimentation rates come from supporting geochronologic and chronostratigraphic data and interpretations based on the depositional system and stratigraphy/sedimentology.

The cyclostratigraphic example used in this tutorial comes from the ~1.4 billion year old Xiamaling Formation and the details of this data set are outlined in Zhang et al. (2015). We will evaluate the Cu/Al data, a paleoenvironmental proxy for productivity/redox state, which comes from a two-meter thick section of rhythmically bedded black shale and chert. This tutorial reproduces the Xiamaling Formation analysis results of Meyers and Malinverno (2018), where you will find additional plots and discussion.

Example R-code

```
# (1) Load the package 'astrochron' (>= version 1.2)
library(astrochron)

# (2) Obtain Xiamaling Cu/Al data, which is built into 'astrochron'.
#     Typically you will use the function 'read' to read your data set
#     into R.
CuAl=getData("Xiamaling-CuAl")

# (3) Interpolate data to a median sampling interval of 0.012 m.
CuAl_0.012=linterp(CuAl)

# (4) Evaluate the data set with 'eha', a time-frequency method.
#     Notice the relatively stable high amplitude cycle at ~20 cycle/m.
eha(CuAl_0.012, win=0.5, step=0.012, pad=500, ydir=-1,genplot=4,pl=2)

# (5) Check on the background continuum using 'periodogram'.
#     This indicates that an AR1 stochastic null model is appropriate
#     for the stratigraphic series, and identifies a cycle exceeding the
#     99% CL (relative to an AR1 null model, with Bonferroni multiple testing
#     correction) at ~20 cycle/m.
periodogram(CuAl_0.012, background=1, bc=T)

# (6) Determine the nominal precession and eccentricity periods at 1.4 Ga,
#     then conduct a nominal timeOpt analysis (see Table S2 of
#     Meyers and Malinverno, 2018).
targetTot=calcPeriods(g=c(5.525000,7.455000,17.300000,17.850000,4.257455),
```

```
k=78,output=2)
targetE=sort(targetTot[1:5],decreasing=T)
targetP=sort(targetTot[6:10],decreasing=T)

# (7) Evaluate the dataset with 'timeOpt'
#     Radioisotopic 207Pb-206Pb data from an overlying 52 m-thick interval
#     of the Xiamaling Formation (unit 2) suggests an average sedimentation
#     rate of 0.66 cm/kyr (99% CI upper bound of 0.92 cm/kyr), but the lower
#     bound is less certain, particularly given that the sedimentology of the
#     analyzed interval (unit 3) is suggestive of a slower accumulation
#     (see discussion in Meyers and Malinverno, 2018, page 9 of supporting
#     info). Here we will investigate all sedimentation rates for which a
#     full astronomical signal can be recovered given the data set
#     resolution (0.2 to 0.5181207 cm/kyr).
timeOpt(CuAl_0.012,sedmin=0.2,sedmax= 0.5181207,numsed=100,targetE=targetE,
targetP=targetP,flow=1/19,fhigh=1/12,roll=10^7,limit=T)

# (8) Evaluate the significance with function 'timeOptSim' via Monte Carlo
#     simulation, using an AR1 null model.  If a power law is more
#     appropriate, use the function 'timeOptSimPwrLaw'.
#     This function call uses 7 cores for parallel processing.
#     The null (AR1) model can be rejected with a high degree of
#     confidence (p-value = 0.005).
timeOptSim(CuAl_0.012,sedmin=0.2,sedmax= 0.5181207,numsed=100,
targetE=targetE,targetP=targetP,flow=1/19,fhigh=1/12,roll=10^7,numsim=2000,
ncores=7)

# (9) Based on the analysis, we conclude that this data set is of high
#     quality and an excellent candidate for TimeOptMCMC.
```

Part 2: Setting up an inversion

Setting up the inversion requires much care, and oftentimes considerable experimentation. There are numerous ways in which the inversion can "go wrong" and produce unreliable results. Therefore, it is necessary to run a series of test analyses prior to moving forward to **Part 3**, to help ensure that the entire solution space is being explored appropriately and the inversion is being conducted correctly. Key steps include defining your priors, setting up the 'jumping parameters' for proposal distributions, and conducting numerous test simulations.

2.1 Setting up your priors. The priors for TimeOptMCMC include the following (Meyers and Malinverno, 2018):

> **Sedimentation rate:** this is modeled as a uniform (uninformative) distribution ranging from `sedmin` to `sedmax`, expressed in units of cm/kyr. The values for these parameters should be based on available geochronologic/chronostratigraphic/depositional-system constraints and the preliminary TimeOpt analyses conducted in **Part 1**.

> **Secular g-frequencies**: these priors are modeled as Gaussian distributions, with a given mean value and standard deviation. Following Meyers and Malinverno (2018) these are based on the simulations of Laskar et al. (2004), with the following values:
> ```
> gAve=c(5.525000,7.455000,17.300000,17.850000,4.257455)
> gSd=c(0.12500,0.01500,0.15000,0.15000,0.00002)
> ```
> In addition, the recent study of Hoang et al. (2021) provides priors for the g frequencies.

Precession constant[2] (k): this is modeled as a Gaussian distribution, with a given mean value and standard deviation. Following Meyers and Malinverno (2018), the estimates from David Waltham's (2015) [model](#) are used based on the expected age of the sediment sequence. The standard deviation is set as half of the total error bounds from that study. Additional priors for k can be found in [the work](#) of Farhat et al. (2022).

Hyperparameters (σ_ϵ and ρ_ϵ): these hyperparameters are required for accurate estimation of the likelihood. The standard deviations σ_ϵ of the spectral and envelope misfits are modeled as $1/\sigma_\epsilon$ distributions, which is appropriate for a scale parameter of the PDF, between a value of $0 < \sigma_\epsilon \leq 1$. The observed data for the spectral and envelope fit are standardized to have unit variance, so that σ_ϵ can be at most 1 (if the observed data contain no astronomical signal). Unit lag correlation coefficients ρ_ϵ of the spectral and envelope misfits are modeled as uniform distributions between a value of $0 \leq \rho_\epsilon < 1$. The parameters should be set as:

```
rhomin=0, rhomax=0.9999, rhostart=-1,
sigmamin=NULL, sigmamax=NULL, sigmastart=1
```

2.2 Setting up the proposal distributions. The Metropolis-Hastings MCMC approach explores the solution space by moving around it in successive 'jumps', evaluating candidate samples with new proposed parameter values. The algorithm will accept the jump under two possible conditions. First, the jump and new candidate values will be accepted if they result in an increased value of the posterior PDF. But even if the posterior PDF is reduced, the algorithm will sometimes accept the jump following a probabilistic rule (see eq. 6 of Meyers and Malinverno, 2018); this ensures that the algorithm has the opportunity to move out of local maxima of the posterior PDF to find the global maximum, and fully explore parameter uncertainty for estimation of the posteriors. The sizes of the jumps are specified using an 'epsilon' value for each of the evaluated parameters (see priors above). You may think of epsilon as analogous to a diffusion coefficient, with larger values allowing for quicker diffusion.

Ideally, we want to make epsilon as large as we reasonably can, to maximize the chance of jumping between possible modes in the solution space. But if we make epsilon too large, acceptance rates for the candidates will plummet. In the most extreme case, the parameter values would not change at all, but more often this would result in needing to run very long MCMC chains to explore the solution space. Alternatively, if we make epsilon too small, nearly all candidates will be accepted, but we won't move far from the initial parameters and fully explore the solution space; again, very long MCMC chains would need to be run in this case. For greatest efficiency in running the algorithm, the percentage of accepted candidates is typically expected to be between 23-44 percent (see Gelman et al., 1996, "Efficient Metropolis jumping rules"). However, the complicated nature of multidimensional parameter spaces may require smaller acceptance rates, and TimeOptMCMC acceptance rates of ~10% can be acceptable.

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[2] Please note that, for consistency with Meyers and Malinverno (2018) and the timeOptMCMC function, the term 'precession constant' is used here for 'k'. In contrast, the updated work of Malinveno and Meyers (2024) uses the term 'precession frequency' or 'axial precession frequency' to refer to 'k'.

One way to go about setting up the jumping parameters is to run a series of TimeOptMCMC analyses in which you sequentially modify the epsilon values for each parameter to get a sense of the sensitivity to each one. An additional approach is to run a coarse resolution analysis (large epsilon) to identify the optimum region, then use as small an epsilon as reasonable to explore that optimum region[3]. In general, this step in the inversion setup can be one of the more time-consuming aspects, and it can sometimes feel like a bit of an artform.

It should be noted that one has the option to specify the initial parameter values used for each MCMC chain, or alternatively, one can have them randomly assigned from the prior distributions. It is generally preferable to randomly initialize the parameter values for each MCMC chain, to avoid getting caught in a 'local maximum'. The one exception is for the sedimentation rate; it can sometimes be useful to set `sedstart` to the r^2_{opt} maximum from the initial TimeOpt analysis (see **Part 1**), but you need to ensure that this is appropriate (see **Part 2.3**).

Figure 1 illustrates some example plots with initial estimates of acceptance rates and stability for an MCMC chain derived from the analysis of the Xiamaling Cu/Al data. A note about 'burn-in' is warranted here. When each MCMC chain is initialized, it will typically require many jumps before it settles into a high-probability region of the posterior PDF (see Figure S3 of Meyers and Malinverno, 2018). This initial portion of the MCMC chain must be identified and discarded prior to using the reliable samples to construct the posterior histogram for each parameter. A standalone function for detecting and removing the burn-in phase is included in **Appendix C** ('burnin'); further details are contained in Meyers and Malinverno (2018).

Example R-code
```
# (1) Load the package 'astrochron' (>= version 1.2)
library(astrochron)

# (2) Obtain Xiamaling Cu/Al data, which is built into 'astrochron'.
#     Typically you will use the function 'read' to read your data set
#     into R.
CuAl=getData("Xiamaling-CuAl")

# (3) Interpolate data to a median sampling interval of 0.012 m.
CuAl_0.012=linterp(CuAl)

# (4) Run a number of short timeOptMCMC chains (3000-5000 samples) to
#     experiment with jumping parameters. A good starting point is to adjust
#     the denominator in epsilon ("20" below), before modifying each
#     parameter individually (if needed). It is useful to view the progress
#     with the option genplot=2 (see Figure 1 for example output).
timeOptMCMC(CuAl_0.012,sedmin=0.1,sedmax=0.6,sedstart=0.33,
gAve=c(5.525000,7.455000,17.300000,17.850000,4.257455),
gSd=c(0.12500,0.01500,0.15000,0.15000,0.00002),gstart=c(-1,-1,-1,-1,-1),
```

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[3] Note that a larger epsilon yields less correlation in MCMC samples. If you want to determine the time constant (thus number of independent samples) associated with a given epsilon, calculate the autocovariance function for accepted samples (post-burn-in). Decimation is useful for generating independent samples if desired. If you run a very long test chain, you can also decimate to conduct a rarefaction analysis (of the parameters).

```
kAve=78,kSd=14,kstart=-1,rhomin=0,rhomax=0.9999, rhostart=-
1,sigmamin=NULL,sigmamax=NULL,sigmastart=1,nsamples=5000,
iopt=1,epsilon=c(0.2,0.2,0.35,0.35,0.8,0.85,0.6,0.35,0.9,0.35,0.9)/20,
ran=T,burnin=-1,output=0,genplot=2,test=F)
```
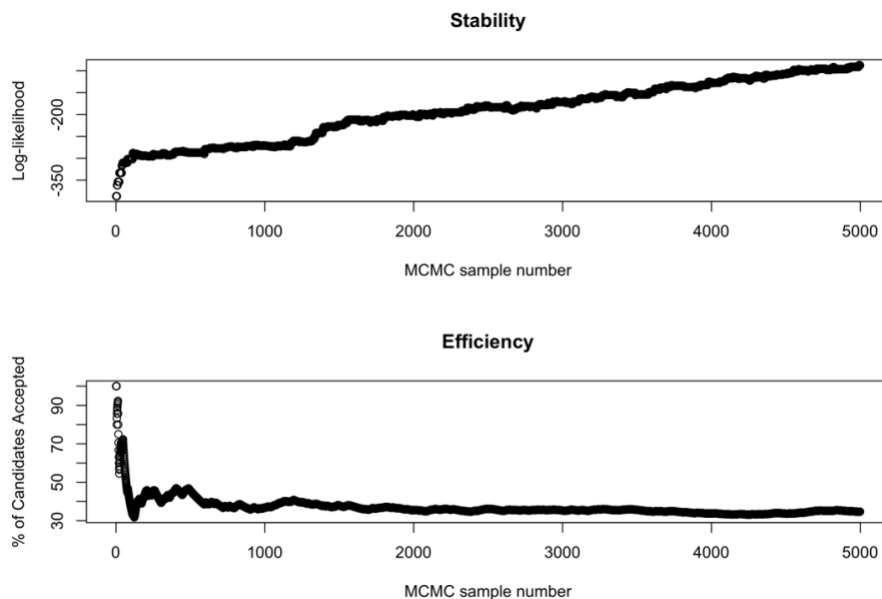
Stability

Efficiency

Figure 1. Some example plots illustrating initial estimates of acceptance rates and stability of the timeOptMCMC results. Note that the log-likelihood continues to increase throughout the analysis, as we are still in the burn-in phase. Acceptance rates typically further decrease following the burn-in phase.

2.3 Inversion quality control. Once you've set up your priors, and believe you have reasonable jumping parameters (epsilons), it is necessary to ensure that the MCMC algorithm is exploring the full parameter space. First, it is important to note that there are different strategies for implementing the MCMC inversion. One can run one long chain, or run multiple short chains and combine them[4].

Determination of the appropriate number of chains and MCMC samples requires experimentation. In general, I have found that it is useful to run many shorter chains (with different random parameter initialization values), to deal with the problem of potentially getting caught in a local-lower-likelihood region of the parameter space. The analysis of the Walvis Ridge data in Meyers & Malinverno (2018) used 150 chains, each with 200,000 MCMC samples, to create stable posteriors. However, to obtain those 150 chains, 200 were run so that chains caught in low likelihood regions could be discarded. The analysis of the Xiamaling Formation data in Meyers and Malinverno (2018) was less challenging (the parameter space was less complicated), so 50 chains could be used, each with 1,000,000 samples. Again, there is a bit of an artform to this assessment. It is reasonable to start with 100 chains of 300,000

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[4] The question of whether it is better to run one long MCMC chain, or numerous short ones is an age-old debate in MCMC. The answer likely depends upon the specific application.

MCMC samples. Your experimentation will be an iterative process, involving numerous inversions (each inversion taking days to possibly weeks).

However, before you run any inversion on your data, it is important to evaluate whether the MCMC algorithm is exploring the full parameter space. To do so, run an analysis with 'test=T', using the total number of MCMC samples (including number of chains) you intend to employ in your cyclostratigraphic data analysis. The 'test=T' option will accept all MCMC candidates. The posterior histogram for each parameter value should approximate the prior distribution. If this is not the case, the epsilon(s) should be increased (see **Part 2.2**) and/or you will need to increase the number of MCMC samples (longer chains and/or more chains). Each test inversion is relatively quick to run and will typically take 5-30 minutes to complete, depending upon your data set, MCMC approach, and computational setup[5]. The results for the code below are shown in **Figure 2**. **Appendix A** and **Appendix B** contain scripts to automate the process.

Example R-code
```
# (1) Load the package 'astrochron' (>= version 1.2)
library(astrochron)

# (2) Obtain Xiamaling Cu/Al data, which is built into 'astrochron'.
#     Typically you will use the function 'read' to read your data set
#     into R.
CuAl=getData("Xiamaling-CuAl")

# (3) Interpolate data to a median sampling interval of 0.012 m.
CuAl_0.012=linterp(CuAl)
# Determine the number of chains and the MCMC chain length you'd like to use.

# (4) Run timeOptMCMC with test=T, to see if you are exploring the full
#     parameter space. If you are using multiple (n) chains, run this n-times
#     and combine the results. See Appendix A for a wrapper function that
#     allows you to automate this. Meyers and Malinverno (2018) used 50
#     chains with 1,000,000 MCMC samples each. It is wise to generate
#     additional chains to compensate for the discarding of chains caught in
#     low likelihood regions, should that occur.
timeOptMCMC(CuAl_0.012,sedmin=0.1,sedmax=0.6,sedstart=0.33,
gAve=c(5.525000,7.455000,17.300000,17.850000,4.257455),
gSd=c(0.12500,0.01500,0.15000,0.15000,0.00002),gstart=c(-1,-1,-1,-1,-1),
kAve=78,kSd=14,kstart=-1,rhomin=0,rhomax=0.9999, rhostart=-
1,sigmamin=NULL,sigmamax=NULL,sigmastart=1,nsamples=1000000,
iopt=1,epsilon=c(0.2,0.2,0.35,0.35,0.8,0.85,0.6,0.35,0.9,0.35,0.9)/20,
ran=T,burnin=-1,output=0,test=T)

# see Appendix B for a script to plot the posteriors for the test analysis.
```

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[5] Reproduction of the entire analysis of the Xiamaling dataset in Parts 2-4 will likely require two-three days on a dedicated computational server, using 10 threads. Reproduction of the analysis of the higher resolution and longer record from Walvis Ridge (Meyers and Malinverno, 2018) will likely require two to three weeks to complete. These two data sets span the length and resolution that one is likely to encounter in most cyclostratigraphic investigations with TimeOptMCMC.
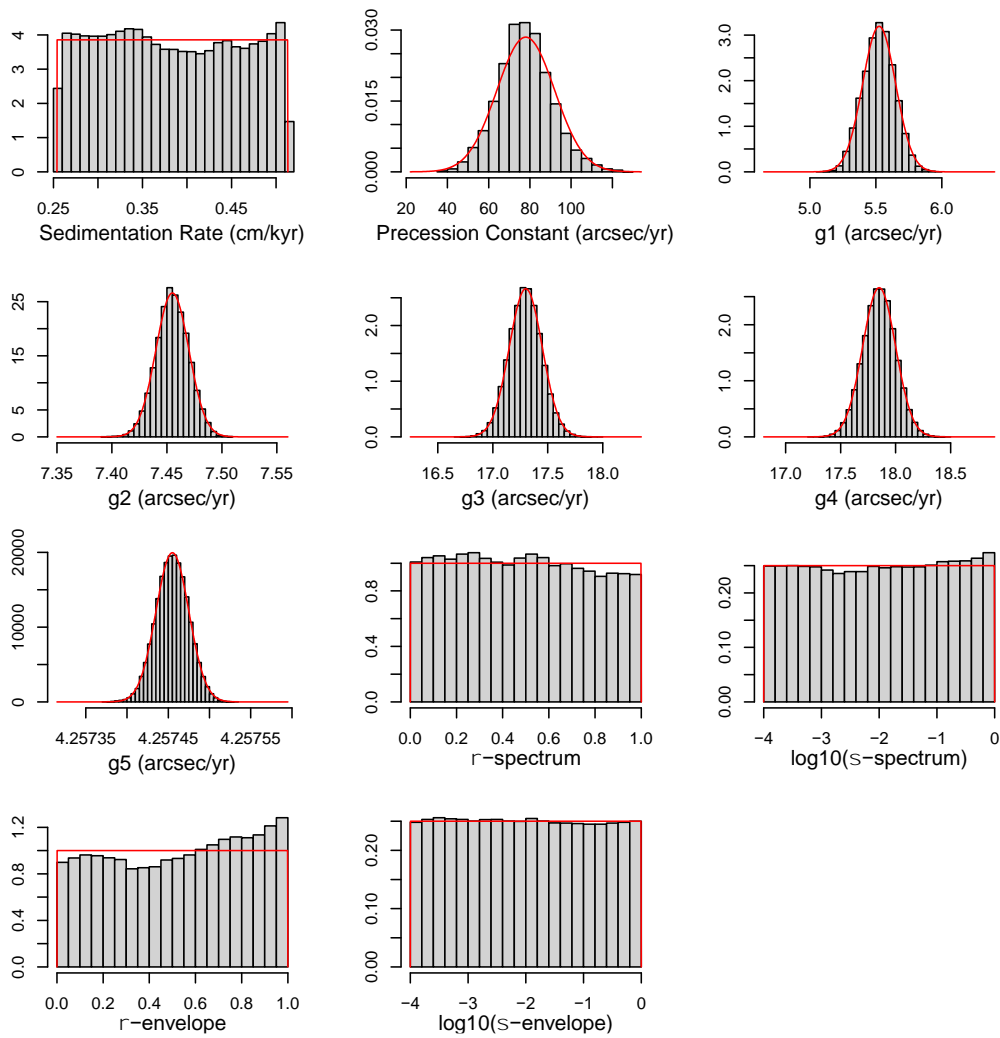
Figure 2. A comparison of the priors (red) and the recovered posteriors (histograms) when all MCMC samples are accepted (option 'test=T'). If these priors and posteriors do not (approximately) match, the MCMC parameters are not adequate to explore the entire parameter space.

Part 3: Executing an inversion

Now that everything is set up, you are ready to complete your first full Bayesian inversion. Note that the first inversion may not be your final one, because it is possible (likely!) that you will learn some things about the algorithm set up and your stratigraphic data series from the results, which will require further adjustment of your analytical approach. But at this point, the task is to initiate the Metropolis-Hastings algorithm, and wait (days to weeks!) for the chains to complete. You will use the same approach as in step 4 of **Part 2**. The wrapper function in **Appendix A** will be helpful if you are running a lot of chains, but be sure to set option 'test=F'. Also, in general, it is a good idea to generate many more chains than you think you'll need, so you can discard those that get stuck in low likelihood regions. **Figure 3** shows results from a Xiamaling MCMC analysis, where some low likelihood chains are observed. Here, 63 chains were MCMC run, 11 of which were trapped in low likelihood regions and discarded prior to estimating the posteriors.
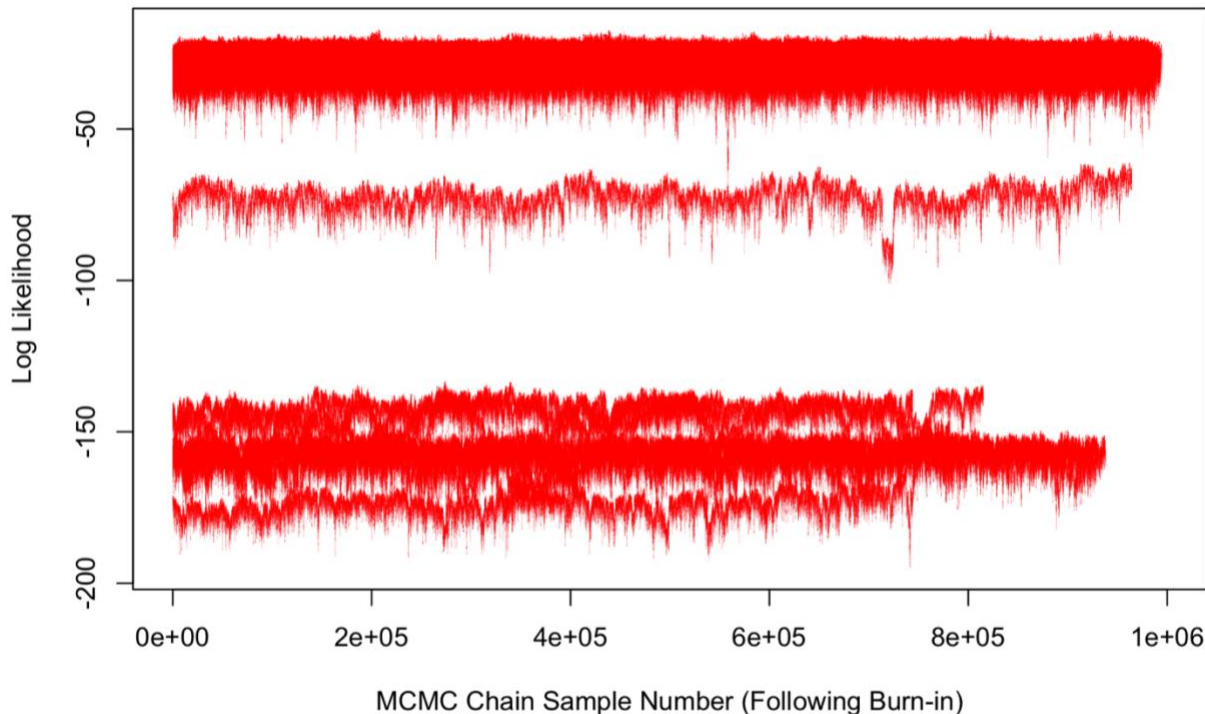
Figure 3. A plot of 63 MCMC chains from an analysis of the Xiamaling Cu/Al data (Meyers and Malinverno, 2018), following burn-in. Note the 11 low likelihood chains (those that are generally less than -50) that should be discarded prior to estimating posteriors. Results from 50 reliable chains at the top of the plot are summarized in the posteriors show in Figures 2A-F, S7 and S8 of Meyers and Malinverno (2018).

You can check on the progress of the inversion by examining the R.out files. You can also evaluate the current status of the posteriors at any point using the script in **Appendix C** (see **Part 4**).

Part 4: Post-processing the results

There are five main steps involved in post-processing your MCMC results:

    (1) The first step is to remove the 'burn-in' interval.

    (2) Then identify any MCMC chains that have gotten stuck in low-likelihood regions of the parameter space (**Figure 3**).

    (3) After you have identified the reliable MCMC chains, they are assembled into a composite of all reliable MCMC samples.

    (4) Use the final composite to estimate posteriors for sedimentation rate, the g-frequencies, the precession constant, and the reconstructed climatic precession and eccentricity frequencies (**Figure 4)**.

    (5) Use the final composite of MCMC samples to estimate posteriors for the Earth-Moon distance and length of day.

        A script for conducting steps 1-4 is in **Appendix C**.

NOTE 4: *In general, satisfactory TimeOptMCMC sampling should result in relatively smooth and (typically) unimodal posterior histograms (see* ***Figure 4****), not overly ragged and/or multimodal distributions. Very ragged posterior histograms typically indicate that not enough MCMC samples have been generated to fully define the posterior PDFs. Multi-modal posterior histograms can indicate that some MCMC chains were caught in low likelihood regions and/or that not enough MCMC samples have been generated.*

If multi-modal posterior histograms persist following correct implementation of the MCMC procedure, they represent ambiguous results with non-unique solutions. For example, an underlying assumption of TimeOptMCMC is that sedimentation rate is relatively constant in the evaluated data series; if this assumption is violated multi-modal behavior can emerge. In that case, it is essential to return to ***Part 1*** *of this document to see if it is possible to identify an interval of relatively stable sedimentation for TimeOptMCMC inversion.*

The following are useful posterior estimates to consider: mean and standard deviation of MCMC samples, maximum a posteriori (MAP) and the 95 percent Credible Interval of MCMC samples.
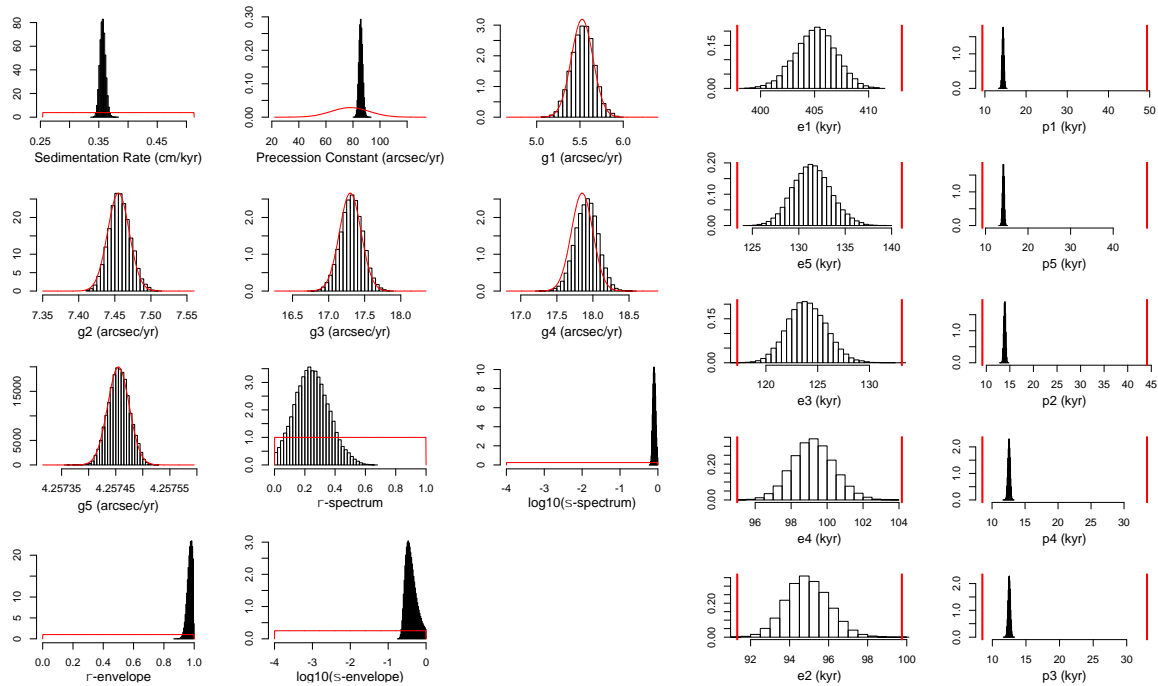
Figure 4. Final TimeOptMCMC posterior distributions for the Xiamaling Cu/Al data, shown as histograms, as reproduced from Figure S7 and S8 of the supplement to Meyers and Malinverno (2018). Red indicates the priors (see Meyers and Malinverno, 2018, for details). Figures copyright (2018) National Academy of Sciences.

Part 5: What should you include in your publication to document correct application of the TimeOptMCMC method?

The following information/plots should ideally be included in your publication to document the TimeOptMCMC analysis, so that the results can be readily evaluated for reliability:

(1) Plots displaying the results of a nominal analysis using TimeOpt, as in Figure S2 of Meyers and Malinverno (2018).

(2) Example MCMC burn-in plot for a single chain, as in Figure S3 of Meyers and Malinverno (2018).

(3) Plots summarizing the evaluation of whether the MCMC algorithm is exploring the full parameter space, as in **Figure 2** of this document.

(4) Plot illustrating the evaluation of all MCMC chains (post burn-in) to identify chains that are trapped in low likelihood regions and should be discarded, as in **Figure 3** of this document.

(5) Report the acceptance rates for the MCMC chains.

(6) Include all supporting scripts used in executing TimeOptMCMC, as in the supplement of Meyers and Malinverno (2018).

(7) And finally, include plots of the priors and posteriors for all parameters (**Figure 4**; Figures S4 and S5 of Meyers and Malinverno, 2018), as well as supporting tables (Table 2 of Meyers and Malinverno, 2018).

For additional information please see Meyers & Malinverno (2018), Meyers (2015), Tarantola (2005), and Malinverno & Briggs (2004).

References

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Appendix A. 'run.R' wrapper

```
# run.R, S.R. Meyers, Feb. 15, 2024
# Save this as run.R, and run it from a terminal by typing
#    R CMD BATCH run.R &
# To check output, type
#    cat run.Rout
# Implement n instances of this script (on n different threads),
# and for each instance create a directory following the format:
#   run_year-month-day_chain_X (X=any other ID information to include)
#     for example, run_22-10-12_01_Xiamaling
# Run each instance from within the given directory
# Use astrochron version 1.2 or greater

library(astrochron)
CuAl=getData("Xiamaling-CuAl")
CuAl_0.012=linterp(CuAl)

timeOptMCMCchain <- function
(dat,iopt=1,chain=1,sedmin=0.5,sedmax=5,sedstart=NULL,gAve=NULL,gSd=NULL,gsta
rt=NULL,kAve=NULL,kSd=NULL,kstart=NULL,rhomin=0,rhomax=0.9999,rhostart=NULL,s
igmamin=NULL,sigmamax=NULL,sigmastart=NULL,ran=F,fit=1,ftol=0.01,roll=10^3,ns
amples=1000,epsilon=NULL,test=F,burnin=-1,detrend=T,verbose=T)
{
  for (i in 1:chain)
    {
res=timeOptMCMC(dat,iopt=1,sedmin=sedmin,sedmax=sedmax,sedstart=sedstart,gAve
=gAve,gSd=gSd,gstart=gstart,kAve=kAve,kSd=kSd,kstart=kstart,rhomin=rhomin,rho
max=rhomax,rhostart=rhostart,sigmamin=sigmamin,sigmamax=sigmamax,sigmastart=s
igmastart,ran=ran,fit=fit,ftol=ftol,roll=roll,nsamples=nsamples,epsilon=epsil
on,test=test,burnin=burnin,detrend=detrend,output=1,savefile=F,genplot=0,verb
ose=verbose)

myfile <-paste("MCMCsamples_",i,".csv",sep="")
write.table(file = myfile, res, sep = ",", row.names = FALSE, append=FALSE)
    }
### END function timeOptMCMCchain
}

# We will run 10 chains with this function call.
# set test=T to test whether the jumping parameters recover the prior.
# set test=F to conduct the inversion.
timeOptMCMCchain(CuAl_0.012,iopt=1,chain=10,sedmin=0.1,sedmax=0.6,sedstart=0.
33, gAve=c(5.525000,7.455000,17.300000,17.850000,4.257455),
gSd=c(0.12500,0.01500,0.15000,0.15000,0.00002),gstart=c(-1,-1,-1,-1,-1),
kAve=78,kSd=14,kstart=-1,rhomin=0,rhomax=0.9999,rhostart=-
1,sigmamin=NULL,sigmamax=NULL,sigmastart=1,nsamples=1000000,
epsilon=c(0.2,0.2,0.35,0.35,0.8,0.85,0.6,0.35,0.9,0.35,0.9)/20,
ran=T,burnin=-1,test=T)

# For a script to read in results and plot posteriors,
#  see Appendix B (test=T) or Appendix C (test=F).

# END run.R
```

Appendix B. 'timeOptMCMC-post-test.R' wrapper to see if your jumping parameters fully explore the priors.

```
# timeOptMCMC-post-test.R, S.R. Meyers, Feb. 15, 2024
# Save this as timeOptMCMC-post-test.R, and run it from a terminal by typing
#   R CMD BATCH timeOptMCMC-post-test.R &
# Run it from the main directory that includes all MCMC subdirectories.
# The resulting plots are saved as timeOptMCMC-test.pdf
#
# This script assumes that you have set up multiple timeOptMCMC analyses,
# in parallel, on multiple processors, and that each instance of timeOptMCMC
# was executed in its own directory (see Appendix A).
# Use astrochron version 1.2 or greater

###########################################################################
# (1) LOAD astrochron PACKAGE, AND SET KEY PARAMETERS
###########################################################################
library(astrochron)


####    SET THE NUMBER OF PROCESSORS HERE:
numproc=5
#####   SET THE NUMBER OF MCMC CHAINS RUN ON EACH PROCESSOR HERE:
numruns=10


# minimum sedimentation rate for investigation in cm/kyr. set sedmin
# and sedmax to the actual minimum and maximum values evaluated
# after accounting for resolution limitations (this was done automatically
# inside the timeOptMCMC function)
sedmin= 0.2539074
# maximum sedimentation rate for investigation in cm/kyr
sedmax= 0.5132661
# average value for the precession constant (arcsec/yr)
kAve=78
# standard deviation for the precession constant (arcsec/yr)
kSd=14
# average g values (arcsec/yr), ordered g1,g2,g3,g4,g5
gAve=c(5.525000,7.455000,17.300000,17.850000,4.257455)
# standard deviation of g values (arcsec/yr), ordered g1,g2,g3,g4,g5
gSd=c(0.12500,0.01500,0.15000,0.15000,0.00002)


#####    - You still need to set each run name ('runame') in section (2).
#####        (You can do this en mass with find/replace function)
#####        The prefixes in section 2 are manually set up for numproc=5.
#####        If you change numproc, you will need to edit the script.
#####    - 'superComp' (section 3) is manually set up for
#####        numproc=5 and numruns=10.  If you change those parameters
#####        the superComp script must be edited.

###########################################################################
# (2) READ ALL MCMC CHAINS.
###########################################################################
cat("\n\n *** READING IN SAMPLES FROM EACH MCMC CHAIN ***\n\n")

if(1 <= numproc)
{
  for(i in 1:numruns)
    {
```

```
    runame = c("run_22-10-12_01_Xiamaling")
    prefix = paste("dat1.", i, sep="")
    cat("\n READING",prefix,"\n")
    assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
  }
}
if(2 <= numproc)
{
  for(i in 1:numruns)
    {
    runame = c("run_22-10-12_02_Xiamaling")
    prefix = paste("dat2.", i, sep="")
    cat("\n READING",prefix,"\n")
    assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
  }
}
if(3 <= numproc)
{
  for(i in 1:numruns)
    {
    runame = c("run_22-10-12_03_Xiamaling")
    prefix = paste("dat3.", i, sep="")
    cat("\n READING",prefix,"\n")
    assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
    }
}
if(4 <= numproc)
{
  for(i in 1:numruns)
    {
    runame = c("run_22-10-12_04_Xiamaling")
    prefix = paste("dat4.", i, sep="")
    cat("\n READING",prefix,"\n")
    assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
    }
}
if(5 <= numproc)
{
  for(i in 1:numruns)
    {
    runame = c("run_22-10-12_05_Xiamaling")
    prefix = paste("dat5.", i, sep="")
    cat("\n READING",prefix,"\n")
    assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
    }
}

##########################################################################
# (3) CREATE superComp
##########################################################################
superComp=rbind(
dat1.1,dat1.2,dat1.3,dat1.4,dat1.5,dat1.6,dat1.7,dat1.8,dat1.9,dat1.10,
```

```
dat2.1,dat2.2,dat2.3,dat2.4,dat2.5,dat2.6,dat2.7,dat2.8,dat2.9,dat2.10,
dat3.1,dat3.2,dat3.3,dat3.4,dat3.5,dat3.6,dat3.7,dat3.8,dat3.9,dat3.10,
dat4.1,dat4.2,dat4.3,dat4.4,dat4.5,dat4.6,dat4.7,dat4.8,dat4.9,dat4.10,
dat5.1,dat5.2,dat5.3,dat5.4,dat5.5,dat5.6,dat5.7,dat5.8,dat5.9,dat5.10
)

superComp=data.frame(superComp)

###########################################################################
# (3b) If this is a really big record, write it out to a file.
###########################################################################
# writeCSV("superComp.csv",superComp)
# afterwards, restart R, and then read it in.
# restartR
# library(astrochron)
# superComp=readMatrix("superComp.csv",check=F,genplot=F)
# superComp=as.data.frame(superComp)
###########################################################################

###########################################################################
# (4) GENERATE SUMMMARY PLOTS FOR g, k, s
###########################################################################
# make a summary figure showing priors vs. MCMC results
histPriorG <- function(dat,ave,sd,true=NULL,xlab,numSd=7)
  {
    grd=seq(ave-numSd*sd,ave+numSd*sd,length=1000)
    den=dnorm(grd,ave,sd)
    histDen=hist(dat[,1],plot=F)
    ylim2=c(0,max(histDen$density,den))
    hist(dat[,1],freq=F,main="",xlab="",ylab="",xlim=c(ave-
numSd*sd,ave+numSd*sd),ylim=ylim2)
    mtext(xlab,side=1,cex=0.8,line=2.3)
    lines(grd,den,lwd=1,col="red")
    polygon(grd,den,col="#FF00004B",border=NA)
# plot true value
    if(!is.null(true)) abline(v=true,col="blue",lty=3,lwd=2)
  }

histPriorU <- function(dat,xmin,xmax,true=NULL,xlab)
  {
    hist(dat[,1],freq=F,main="",xlab="",ylab="",xlim=c(xmin,xmax))
    mtext(xlab,side=1,cex=0.8,line=2.3)
    grd=seq(xmin,xmax,length=1000)
    den=dunif(grd,xmin,xmax)
# modify the first and last to go to zero, to plot a box
    den[1]=0
    den[1000]=0
    lines(grd,den,lwd=1,col="red")
    polygon(grd,den,col="#FF00004B",border=NA)
# plot true value
    if(!is.null(true)) abline(v=true,col="blue",lty=3,lwd=2)
  }

pl(r=4,c=3,mar=c(3.1, 3.1, 2.1, 2.1),file="timeOptMCMC-test.pdf")
histPriorU(superComp[2],xmin=sedmin,xmax=sedmax,xlab="Sedimentation Rate
(cm/kyr)")
```

```
histPriorG(superComp[3],ave=kAve,sd=kSd,xlab="Precession Constant
(arcsec/yr)",numSd=4)
histPriorG(superComp[4],ave=gAve[1],sd=gSd[1],xlab="g1 (arcsec/yr)")
histPriorG(superComp[5],ave=gAve[2],sd=gSd[2],xlab="g2 (arcsec/yr)")
histPriorG(superComp[6],ave=gAve[3],sd=gSd[3],xlab="g3 (arcsec/yr)")
histPriorG(superComp[7],ave=gAve[4],sd=gSd[4],xlab="g4 (arcsec/yr)")
histPriorG(superComp[8],ave=gAve[5],sd=gSd[5],xlab="g5 (arcsec/yr)")
histPriorU(superComp[9],xmin=0,xmax=1,xlab=expression(paste(rho,"-
spectrum")))
histPriorU(log10(superComp[10]),xmin=log10(1e-
04),xmax=log10(1),xlab=expression(paste("log10(",sigma,"-spectrum)")))
histPriorU(superComp[11],xmin=0,xmax=1,xlab=expression(paste(rho,"-
envelope")))
histPriorU(log10(superComp[12]),xmin=log10(1e-
04),xmax=log10(1),xlab=expression(paste("log10(",sigma,"-envelope)")))

dev.off()
# END timeOptMCMC-post-test.R
```

Appendix C. timeOptMCMC-post.R wrapper for post-processing and plotting posteriors

```
# timeOptMCMC-post.R, S.R. Meyers, Feb. 15, 2024

# Run this interactively (not as a batch script).
# This script assumes that you have set up multiple timeOptMCMC analyses,
# in parallel, on multiple processors, and that each instance of timeOptMCMC
# was executed in its own directory (see Appendix A).
#
# I typically let those analyses run for a few days to weeks (depending
# on the data set), to help ensure that there are enough valid MCMC chains,
# after discarding those that clearly are trapped in low likelihood regions
# (their likelihoods are many orders of magnitude lower than the best
# fitting results). usually, I do not bother to let it run to
# completion. The basic idea is to have more MCMC chains than you need when
# it comes time for post-processing.
#
# The way to use this script is to set the number of runs (numruns) x
# number of processors (numproc) to the maximum total number of chains that
# you want to evaluate. Start small, and add more as needed...
# Use astrochron version 1.2 or greater

#############################################################################
# (1) READ LIBRARIES and functions, set parameters
#############################################################################
library(astrochron)

# below is a function to remove burnin interval, S.R. Meyers, 2017
# paste it into the R console
      burnin <- function(dat,nburnin=-1,decimate=1)
       {
      # dat = matrix or data frame with your MCMC samples. first column
      #  must be log-likelihood
      # nburnin= define number of initial points to discard. if <0,
      #  will use criterion from Alberto Malinverno
      # decimate= downsample every x samples

      # MCMC samples
         dat=data.frame(dat)
         npts=length(dat[,1])
         iml = which.max(dat[,1])
         logpdfmap = dat[iml,1]
      # burn in detection, using median value from second half of samples
         if(nburnin<0)
          {
            logpdfburnin=median(dat[(npts/2):npts,1])
      # identify the first value to go above it
            nburnin=which(dat[,1]>logpdfburnin)[1]
          }
      # remove burnin interval
         dat2=dat[(nburnin+1):npts,]
         npts2=length(dat2[,1])
      # now decimate if desired
         if(decimate>1)
          {
            dat3=dat2[seq(1, length(dat2[,1]), decimate),]
            npts3=length(dat3[,1])
```

```
             if(verbose) cat("* Number of samples after
        decimation=",npts3,"\n")
              }
              if(decimate == 1) return(dat2)
              if(decimate > 1) return(dat3)
        # end function burnin
        }

####    SET THE NUMBER OF PROCESSORS HERE:
numproc=5
#####    SET THE NUMBER OF MCMC CHAINS RUN ON EACH PROCESSOR HERE:
numruns=10

# minimum sedimentation rate for investigation in cm/kyr. set sedmin
# and sedmax to the actual minimum and maximum values evaluated
# after accounting for resolution limitations (this was done automatically
# inside the timeOptMCMC function)
sedmin= 0.2539074
# maximum sedimentation rate for investigation in cm/kyr
sedmax= 0.5132661
# average value for the precession constant (arcsec/yr)
kAve=78
# standard deviation for the precession constant (arcsec/yr)
kSd=14
# average g values (arcsec/yr), ordered g1,g2,g3,g4,g5
gAve=c(5.525000,7.455000,17.300000,17.850000,4.257455)
# standard deviation of g values (arcsec/yr), ordered g1,g2,g3,g4,g5
gSd=c(0.12500,0.01500,0.15000,0.15000,0.00002)


#####    - You still need to set each run name ('runame') in section (2).
#####       (You can do this en mass with find/replace function)
#####       The prefixes in section 2 are manually set up for numproc=5.
#####       If you change numproc, you will need to edit the script.
#####    - You must MANUALLY SET 'ylimMin' and 'ylimMax' (section 4) below.
#####    - 'superComp' (section 5) is manually set up for numproc=5
#####       and numruns=10.  If you change those parameters the superComp
#####       script must be edited.
#####    - Finally, you must set the true values appropriately if known
#####       (section 7).


############################################################################
# (2) READ ALL MCMC CHAINS.
############################################################################
cat("\n\n *** READING IN SAMPLES FROM EACH MCMC CHAIN ***\n\n")

if(1 <= numproc)
{
  for(i in 1:numruns)
    {
      runame = c("run_22-10-12_01_Xiamaling")
      prefix = paste("dat1.", i, sep="")
      cat("\n READING",prefix,"\n")
      assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
    }
```

```r
}
if(2 <= numproc)
{
  for(i in 1:numruns)
    {
      runame = c("run_22-10-12_02_Xiamaling")
      prefix = paste("dat2.", i, sep="")
      cat("\n READING",prefix,"\n")
      assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
    }
}
if(3 <= numproc)
{
  for(i in 1:numruns)
    {
      runame = c("run_22-10-12_03_Xiamaling")
      prefix = paste("dat3.", i, sep="")
      cat("\n READING",prefix,"\n")
      assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
    }
}
if(4 <= numproc)
{
  for(i in 1:numruns)
    {
      runame = c("run_22-10-12_04_Xiamaling")
      prefix = paste("dat4.", i, sep="")
      cat("\n READING",prefix,"\n")
      assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
    }
}
if(5 <= numproc)
{
  for(i in 1:numruns)
    {
      runame = c("run_22-10-12_05_Xiamaling")
      prefix = paste("dat5.", i, sep="")
      cat("\n READING",prefix,"\n")
      assign(prefix ,readMatrix(paste(runame,"/MCMCsamples_",i,".csv",
sep=""),check=F,genplot=F))
    }
}

############################################################################
# (3) REMOVE BURN-IN AND EXTRACT g, k, s
############################################################################
cat("\n\n *** BURNING-IN TO EXTRACT G,K,S ***\n\n")
for(j in 1:numproc)
 {
    for(i in 1:numruns)
      {
        cat("\n")
        now=get(print(paste("dat",j,".", i, sep="")))
        prefix = paste("dat",j,".", i, "B", sep="")
```

```r
        assign(prefix , burnin(now,nburnin=-1))
    }
}


########################################################################
# (4) PLOT LOGLIKELIHOODS FOR EACH CHAIN
########################################################################
#####  MANUALLY SET  #####
ylimMin=min(
dat1.1B[,1],dat1.2B[,1],dat1.3B[,1],dat1.4B[,1],dat1.5B[,1],
dat1.6B[,1],dat1.7B[,1],dat1.8B[,1],dat1.9B[,1],dat1.10B[,1],
dat2.1B[,1],dat2.2B[,1],dat2.3B[,1],dat2.4B[,1],dat2.5B[,1],
dat2.6B[,1],dat2.7B[,1],dat2.8B[,1],dat2.9B[,1],dat2.10B[,1],
dat3.1B[,1],dat3.2B[,1],dat3.3B[,1],dat3.4B[,1],dat3.5B[,1],
dat3.6B[,1],dat3.7B[,1],dat3.8B[,1],dat3.9B[,1],dat3.10B[,1],
dat4.1B[,1],dat4.2B[,1],dat4.3B[,1],dat4.4B[,1],dat4.5B[,1],
dat4.6B[,1],dat4.7B[,1],dat4.8B[,1],dat4.9B[,1],dat4.10B[,1],
dat5.1B[,1],dat5.2B[,1],dat5.3B[,1],dat5.4B[,1],dat5.5B[,1],
dat5.6B[,1],dat5.7B[,1],dat5.8B[,1],dat5.9B[,1],dat5.10B[,1]
)

#####  MANUALLY SET  #####
ylimMax=max(
dat1.1B[,1],dat1.2B[,1],dat1.3B[,1],dat1.4B[,1],dat1.5B[,1],
dat1.6B[,1],dat1.7B[,1],dat1.8B[,1],dat1.9B[,1],dat1.10B[,1],
dat2.1B[,1],dat2.2B[,1],dat2.3B[,1],dat2.4B[,1],dat2.5B[,1],
dat2.6B[,1],dat2.7B[,1],dat2.8B[,1],dat2.9B[,1],dat2.10B[,1],
dat3.1B[,1],dat3.2B[,1],dat3.3B[,1],dat3.4B[,1],dat3.5B[,1],
dat3.6B[,1],dat3.7B[,1],dat3.8B[,1],dat3.9B[,1],dat3.10B[,1],
dat4.1B[,1],dat4.2B[,1],dat4.3B[,1],dat4.4B[,1],dat4.5B[,1],
dat4.6B[,1],dat4.7B[,1],dat4.8B[,1],dat4.9B[,1],dat4.10B[,1],
dat5.1B[,1],dat5.2B[,1],dat5.3B[,1],dat5.4B[,1],dat5.5B[,1],
dat5.6B[,1],dat5.7B[,1],dat5.8B[,1],dat5.9B[,1],dat5.10B[,1]
)

# plot a summary of the MCMC chains post-burnin
chainlength=length(dat1.1[,1])
pl(r=1,c=1,h=5.5,w=8)
ylim=c(ylimMin,ylimMax)
plot(dat1.1B[,1],type="l",ylim=ylim,xlim=c(1,chainlength),ylab="Log
Likelihood",xlab="MCMC Chain Sample Number (Following Burn-in)",main="Summary
of MCMC Samples From Each Chain",col="red",lwd=0.1)
cat("dat1.1B log-likelihood MAX==",max(dat1.1B[,1]),"\n")
cat("dat1.1B log-likelihood MIN==",min(dat1.1B[,1]),"\n\n")
for(j in 1:numproc)
 {
   for(i in 1:numruns)
     {
       now=get(print(paste("dat",j,".", i,"B", sep="")))[,1]
       cat(paste("dat1.", i,"B log-likelihood MAX= ",max(now), sep=""),"\n")
       cat(paste("dat1.", i,"B log-likelihood MIN = ",min(now),
sep=""),"\n\n")
       lines(now,col="red",lwd=0.1)
     }
 }
```

```
#############################################################################
# (5) BASED ON LOGLIKELIHOOD PLOTS FOR EACH CHAIN, IDENTIFY THOSE TO REMOVE
#     AND MAKE YOUR FINAL 'superComp'
#############################################################################
# REMOVE chains where likelihood is orders of magnitude lower than the others

#####  MANUALLY SET  #####
superComp=rbind(
dat1.1B,dat1.2B,dat1.3B,dat1.4B,dat1.5B,
dat1.6B,dat1.7B,dat1.8B,dat1.9B,dat1.10B,
dat2.1B,dat2.2B,dat2.3B,dat2.4B,dat2.5B,
dat2.6B,dat2.7B,dat2.8B,dat2.9B,dat2.10B,
dat3.1B,dat3.2B,dat3.3B,dat3.4B,dat3.5B,
dat3.6B,dat3.7B,dat3.8B,dat3.9B,dat3.10B,
dat4.1B,dat4.2B,dat4.3B,dat4.4B,dat4.5B,
dat4.6B,dat4.7B,dat4.8B,dat4.9B,dat4.10B,
dat5.1B,dat5.2B,dat5.3B,dat5.4B,dat5.5B,
dat5.6B,dat5.7B,dat5.8B,dat5.9B,dat5.10B
)

# let's look again, after removing the extremely poor fits
pl(r=1,c=1,h=5.5,w=8)
plot(superComp[,1],type="l",ylab="Log Likelihood",xlab="MCMC Chain Sample
Number",main="Final MCMC Samples Assembled From Each chain",
col="red",lwd=0.1)

#############################################################################
# STEP (5a) If this is a really big record, write it out to a file.
#############################################################################
writeCSV("superComp.csv",superComp)
# afterwards, restart R to clean out the buffers, and then read it in.
# restartR
# library(astrochron)
# superComp=readMatrix("superComp.csv",check=F,genplot=F)
# superComp=as.data.frame(superComp)
#############################################################################

#############################################################################
# (6) CALCULATE SUMMARY STATISTICS FOR g, k, s
#############################################################################
# average for each posterior
colMeans(superComp)
# standard deviation for each posterior
apply(superComp,2,sd)

#############################################################################
# (7) GENERATE SUMMMARY PLOTS FOR g, k, s
#############################################################################
# make a summary figure showing priors vs. MCMC results
histPriorG <- function(dat,ave,sd,true=NULL,xlab,numSd=7)
  {
    grd=seq(ave-numSd*sd,ave+numSd*sd,length=1000)
    den=dnorm(grd,ave,sd)
    histDen=hist(dat[,1],plot=F)
    ylim2=c(0,max(histDen$density,den))
    hist(dat[,1],freq=F,main="",xlab="",ylab="",xlim=c(ave-
numSd*sd,ave+numSd*sd),ylim=ylim2)
```

```r
    mtext(xlab,side=1,cex=0.8,line=2.3)
    lines(grd,den,lwd=1,col="red")
    polygon(grd,den,col="#FF00004B",border=NA)
# plot true value
    if(!is.null(true)) abline(v=true,col="blue",lty=3,lwd=2)
  }

histPriorU <- function(dat,xmin,xmax,true=NULL,xlab)
  {
    hist(dat[,1],freq=F,main="",xlab="",ylab="",xlim=c(xmin,xmax))
    mtext(xlab,side=1,cex=0.8,line=2.3)
    grd=seq(xmin,xmax,length=1000)
    den=dunif(grd,xmin,xmax)
# modify the first and last to go to zero, to plot a box
    den[1]=0
    den[1000]=0
    lines(grd,den,lwd=1,col="red")
    polygon(grd,den,col="#FF00004B",border=NA)
# plot true value
    if(!is.null(true)) abline(v=true,col="blue",lty=3,lwd=2)
  }

pl(r=4,c=3,mar=c(3.1, 3.1, 2.1, 2.1))
histPriorU(superComp[2],xmin=sedmin,xmax=sedmax,xlab="Sedimentation Rate
(cm/kyr)")
histPriorG(superComp[3],ave=kAve,sd=kSd,xlab="Precession Constant
(arcsec/yr)",numSd=4)
histPriorG(superComp[4],ave=gAve[1],sd=gSd[1],xlab="g1 (arcsec/yr)")
histPriorG(superComp[5],ave=gAve[2],sd=gSd[2],xlab="g2 (arcsec/yr)")
histPriorG(superComp[6],ave=gAve[3],sd=gSd[3],xlab="g3 (arcsec/yr)")
histPriorG(superComp[7],ave=gAve[4],sd=gSd[4],xlab="g4 (arcsec/yr)")
histPriorG(superComp[8],ave=gAve[5],sd=gSd[5],xlab="g5 (arcsec/yr)")
histPriorU(superComp[9],xmin=0,xmax=1,xlab=expression(paste(rho,"-
spectrum")))
histPriorU(log10(superComp[10]),xmin=log10(1e-
04),xmax=log10(1),xlab=expression(paste("log10(",sigma,"-spectrum)")))
histPriorU(superComp[11],xmin=0,xmax=1,xlab=expression(paste(rho,"-
envelope")))
histPriorU(log10(superComp[12]),xmin=log10(1e-
04),xmax=log10(1),xlab=expression(paste("log10(",sigma,"-envelope)")))

########################################################################
# (8) EVALUATE PRECESSION AND ECCENTRICITY PERIODS
########################################################################
cat("\n\n *** DETERMINING ASTRONOMICAL PERIODS ***\n\n")
superDat=calcPeriods(g=cbind(superComp[,4],superComp[,5],superComp[,6],superC
omp[,7],superComp[,8]),k=superComp[,3])

########################################################################
# (9) CALCULATE SUMMARY STATISTICS FOR PRECESSION AND ECCENTRICITY PERIODS
########################################################################
# average periods for each posterior
colMeans(superDat)

# standard deviation of periods for each posterior
apply(superDat,2,sd)
```

```r
# average frequency for each posterior
colMeans(1/superDat)

# EQUIVALENT PERIODS:
1/colMeans(1/superDat)

# standard deviation of frequencies for each posterior
apply(1/superDat,2,sd)

############################################################################
# (10) GENERATE SUMMMARY PLOTS FOR PRECESSION AND ECCENTRICITY PERIODS
############################################################################
# make a summary figure showing max and min possible periods & MCMC results
minP <- function(gAve,gSd,kAve,kSd,sigma=4)
  {
        e1min=1296/((gAve[2]+sigma*gSd[2])-(gAve[5]-sigma*gSd[5]))
        e2min=1296/((gAve[4]+sigma*gSd[4])-(gAve[5]-sigma*gSd[5]))
        e3min=1296/((gAve[4]+sigma*gSd[4])-(gAve[2]-sigma*gSd[2]))
        e4min=1296/((gAve[3]+sigma*gSd[3])-(gAve[5]-sigma*gSd[5]))
         e5min= 1296/((gAve[3]+sigma*gSd[3])-(gAve[2]-sigma*gSd[2]))
        p1min=1296/((kAve+sigma*kSd)+(gAve[5]+sigma*gSd[5]))
        p2min= 1296/((kAve+sigma*kSd)+(gAve[2]+sigma*gSd[2]))
        p3min= 1296/((kAve+sigma*kSd)+(gAve[4]+sigma*gSd[4]))
        p4min= 1296/((kAve+sigma*kSd)+(gAve[3]+sigma*gSd[3]))
        p5min= 1296/((kAve+sigma*kSd)+(gAve[1]+sigma*gSd[1]))
        minP=c(e1min,e5min,e3min,e4min,e2min,p1min,p5min,p2min,p4min,p3min)
        return(minP)
  }

maxP <- function(gAve,gSd,kAve,kSd,sigma=4)
  {
        e1max=1296/((gAve[2]-sigma*gSd[2])-(gAve[5]+sigma*gSd[5]))
        e2max=1296/((gAve[4]-sigma*gSd[4])-(gAve[5]+sigma*gSd[5]))
        e3max=1296/((gAve[4]-sigma*gSd[4])-(gAve[2]+sigma*gSd[2]))
        e4max=1296/((gAve[3]-sigma*gSd[3])-(gAve[5]+sigma*gSd[5]))
         e5max= 1296/((gAve[3]-sigma*gSd[3])-(gAve[2]+sigma*gSd[2]))
        p1max=1296/((kAve-sigma*kSd)+(gAve[5]-sigma*gSd[5]))
        p2max= 1296/((kAve-sigma*kSd)+(gAve[2]-sigma*gSd[2]))
        p3max= 1296/((kAve-sigma*kSd)+(gAve[4]-sigma*gSd[4]))
        p4max= 1296/((kAve-sigma*kSd)+(gAve[3]-sigma*gSd[3]))
        p5max= 1296/((kAve-sigma*kSd)+(gAve[1]-sigma*gSd[1]))
        maxP=c(e1max,e5max,e3max,e4max,e2max,p1max,p5max,p2max,p4max,p3max)
        return(maxP)
  }

pMin=minP(gAve=gAve,gSd=gSd,kAve=kAve,kSd=kSd)
pMax=maxP(gAve=gAve,gSd=gSd,kAve=kAve,kSd=kSd)


histPeriods <- function(dat,xmin,xmax,true=NULL)
  {
    hist(dat[,1],freq=F,main="",xlab="",ylab="",xlim=c(xmin,xmax))
    mtext(paste(colnames(dat),"(kyr)"),side=1,cex=0.8,line=2.3)
    abline(v=c(xmin,xmax),lwd=2,col="red")
    if(!is.null(true)) abline(v=true,col="blue",lty=3,lwd=2)
  }
```

```
# periods=gsk(g=c(5.59,7.452,17.368,17.916,4.257452),k=50.4844)[1:10,1]
# sort(periods,decreasing=T)

pl(r=5,c=2,mar=c(3.4, 3.1, 2.1, 2.1),w=5,h=7)
histPeriods(superDat[1],xmin=pMin[1],xmax=pMax[1])
histPeriods(superDat[6],xmin=pMin[6],xmax=pMax[6])

histPeriods(superDat[2],xmin=pMin[2],xmax=pMax[2])
histPeriods(superDat[7],xmin=pMin[7],xmax=pMax[7])

histPeriods(superDat[3],xmin=pMin[3],xmax=pMax[3])
histPeriods(superDat[8],xmin=pMin[8],xmax=pMax[8])

histPeriods(superDat[4],xmin=pMin[4],xmax=pMax[4])
histPeriods(superDat[9],xmin=pMin[9],xmax=pMax[9])

histPeriods(superDat[5],xmin=pMin[5],xmax=pMax[5])
histPeriods(superDat[10],xmin=pMin[10],xmax=pMax[10])


# without bounds
pl(r=5,c=2,mar=c(3.4, 3.1, 2.1, 2.1),w=5,h=7)
hist(superDat[,1],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[1]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,6],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[6]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,2],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[2]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,7],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[7]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,3],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[3]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,8],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[8]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,4],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[4]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,9],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[9]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,5],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[5]),"(kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,10],freq=F,main="",xlab="",ylab="")
mtext(paste(colnames(superDat[10]),"(kyr)"),side=1,cex=0.8,line=2.3)


# for a view of the frequencies
superDat=1/superDat

pl(r=5,c=2,mar=c(4.1, 3.1, 3.1, 2.1),w=5,h=7)
```

```r
hist(superDat[,1],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[1]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,2],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[2]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,3],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[3]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,4],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[4]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,5],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[5]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,6],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[6]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,7],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[7]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,8],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[8]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,9],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[9]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

hist(superDat[,10],main="",xlab="",ylab="")
mtext(paste(colnames(superDat[10]),"(1/kyr)"),side=1,cex=0.8,line=2.3)

# END timeOptMCMC-post.R
```