A guide for Bayesian analysis in ADMB

Cole C. Monnahan — monnahc@uw.edu

August 7, 2014

Abstract

The point of this document is.....

Contents

1	Bay	Bayesian inference			
	1.1	Priors	[
2	Mar	rkov cl	hain Monte Carlo		
	2.1	Workf	low		
	2.2	MCM	C Phases		
	2.3	Outpu	it files		
		2.3.1	Meta data: The hst file		
		2.3.2	Parameter draws: The psv file		
		2.3.3	Derived quantity draws		
	2.4	Restar	rting a chain		
	2.5		ergence diagnostics		
	2.6		ng values and scaling		
	2.7		polis-Hastings		
		2.7.1	Algorithm		
		2.7.2	MCMC Arguments		
		2.7.3	mcprobe		
		2.7.4	mcrb		
		2.7.5	Example MCMC		
		2.7.6	User-supplied correlation matrix		
	2.8		d		
	2.0	2.8.1	Algorithm		
		2.8.2			
			0		
		2.8.3	Tuning the hybrid algorithm		

1 Bayesian inference

In general, Bayesian inference is used to quantify the full range of uncertainty around both models and parameter values and incorporate findings from historical studies. In a fisheries specific context, Bayesian inference allows scientists to investigate the consequences of alternative management strategies.

2 MCMC

Markov chain Monte Carlo (MCMC) is a common algorithm used to sample and compute expectations with respect to complex and high-dimensional probability distributions. ADMB implements two different MCMC

algorithms: the ubiqitous Metropolis-Hastings and a Hamiltonian (or "hybrid") sampler, both described in this section.

John Kruschke in "Doing Bayesian Data Analysis: A Tutorial with R and BUGS" has a simple example that illustrates the mechanics of the Metropolis-Hastings algorithm. A politician lives on a long chain of islands. The politician's goal is to stay in the public eye by traveling to each island proportional to their relative population. In other words, he will spend more time on highly populated islands and less time on less populated islands. He flips a fair coin to propose a move to an island east or west of his current location. If the proposed island has a higher population than his current island he moves. If the proposed island has a smaller population than his current island he will only move with a probability $P_{proposed}/P_{current}$ where $P_{proposed}$ is the population of the proposed island and $P_{current}$ is the population of the current island.

All MCMC algorithms work in this same general way. The user will start the algorithm at an arbitrary starting point, and the algorithm will propose new parameter sets or states. The algorithm will propose new states (i.e. parameter draws) and move to that state, or not, depending on its density relative to the current state. Just like the politician, the algorithm will spend most of the time in states with high densities.

MCMC algorithms typically need a "burn-in" period, especially if the starting point is in a region with low density. The goal of a MCMC algorithm is to explore areas with the highest probabilities in a distribution. It will perhaps take thousands of draws for the algorithm to find the peaks of the distribution, especially if it starts in a low density region. Discarding these intial draws allows the algorithm to explore the main regions of the target distribution.

Autocorrelated MCMC samples are close together and probably not a true representation of the underlying distribution. Samples are typically "thinned" every nth-step to generate uncorrelated samples. The tradeoff is that excessive thinning increases run-time for the algorithm.

The R package CODA is a commonly used tool for checking MCMC diagnostics such as autocorrelation.

2.1 Priors

As with any Bayesian analysis, priors are a key component of the posterior surface and must be considered in ADMB as well. The posterior density is proportional to the product of the likelihood and priors. ADMB works in the negative log space, so he contribution of priors is incorporated into the model by adding the negative log of the prior density to the objective function. At this point the minimum point is no longer the maximum likelihood estimate, but rather what we refer to as the "maximum posterior mode"— i.e. the parameters corresponding to the highest point of the posterior. The difference between the two is subtle, but there are important philosophical differences: with Bayesian analysis ADMB is integrating across the parameter space, while the likelihood framework focuses on maximization.

The way MCMC works in ADMB, users need not explicitly define and incorporate priors into their model. In this case "implicit" priors are still affecting the posterior. In particular, unbounded parameters without explicit priors have infinitely broad uniform priors (an example of an "improper" prior because it will not integrate to 1). Another example is a variance parameter estimated in log space and then exponentiated within the model to keep it above zero. An implicit uniform prior on the log parameter may not be uninformative on the natural scale. The implications of these issues are contentious and certainly beyond the scope of this guide. We caution users to carefully consider and explicitly acknowledge their priors – ADMB will not force you to.

Uniform priors can be incorporated without changing the objective function calculation by bounding the parameter. Other forms of prior distributions need to be added manually by the user, with our without any constants. For instance, a normal (N(5,1)) prior on a parameter a could be added as f+=pow((a-5),2)/(2*1*1), where the constants have been dropped.

3 Markov chain Monte Carlo

Markov chain Monte Carlo (MCMC) is a common algorithm used to sample from arbitrary, unscaled posterior distributions. ADMB implements two different MCMC algorithms: the ubiquitous Metropolis-Hastings and a Hamiltonian (or "hybrid") sampler, both described briefly below.

All MCMC algorithms work by proposing new states (i.e. parameter vectors) and moving to that state, or not, depending on its density relative to the current state. The algorithm thus generates series of au-

to correlated parameter vectors which can be thinned to produce independent samples from the posterior distribution of interest.

3.1 Workflow

The following steps outline the basic workflow typically used for conducting a MCMC in ADMB.

- 1. Build, run, and verify an ADMB model. This model must explicitly include the contribution of the priors to the objective function, such that the ADMB estimate is the posterior mode, rather than a maximum likelihood estimate.
- 2. Run an MCMC using the command line argument -mcmc N -mcsave N_{save} (among other options, see below). The thinned draws are discarded, leaving a total of $N_{\text{out}} = N/N_{\text{save}}$ saved draws. For example -mcmc 1e6 -mcsave 1000 will run 1 million draws but only save (i.e. "thin") every 1000th, for a total kept of Nout = 1000.
- 3. After completion, run the model again with argument -mceval. This command tells ADMB to loop through the saved iterations (in the .psv file) and execute in the mceval_phase().
- 4. Pull results into R or other program to ensure the sample is sufficiently thinned, either visually or with tools using, for example, the CODA package.
- 5. If necessary, rerun the chain with more thinning, drop the first part of the chain as a "burn-in," or run longer for more iterations.
- 6. Make whatever Bayesian inference is desired using the *Nout* independent samples.

3.2 MCMC Phases

ADMB is designed with two phases that are used to produce MCMC output: (1) the mcmc phase and (2) mceval phase. While the use of these phases is not common (is this true??) among other MCMC software, and may be a source of confusion for new ADMB users, they provide a powerful and efficient framework for MCMC analyses.

The mcmc phase is the one with which most people are already familiar. This is where ADMB generates new parameter sets by proposing a set, and then determining whether to move there or stay at the current set. This process is repeated N times, and how sets are proposed depend on the algorithm used (see section 2.7 and 2.8). During this phase, the Nout saved parameter values are written to a .psv file (described below). Note that if -mcsave nsave is not specified, ADMB will run the MCMC but no values will be saved

The mceval is an optional phase that is designed to be run after the .psv file has been produced. During this phase, ADMB loops through the *Nout* parameter combinations in the .psv file and reruns the PROCEDURE_SECTION in the mceval() phase. This phase is extremely powerful because it allows the user to minimize wasted calculations by parsing calculations into two groups: those that affect the objective function (i.e. posterior calculations for Bayesian analyses) and those that do not. Calculations done for discarded draws (which often is most iterations) simply slow down the analysis. Thus, an analysis can be made to run faster by minimizing calculations in the mcmc phase. For example, a user may want to extrapolate (e.g. project a time series into the future) or calculate values derived from the parameters and intermediate values. By putting these calculations inside an mceval_phase clause they are only done for saved draws and the MCMC will run faster. In practice, some chains need to be thinned significantly more than 1 in 1000, so the time saved can be substantial, especially if the mceval_phase calculations are time-consuming.

While the mceval phase was designed specifically for MCMC analyses, it can be coopted for use in other types of analyses. In essence it is a convenient framework in which to get ADMB to quickly evaluate arbitrary sets of parameters, while only initializing once. Examples of alternative uses are the SIR algorithm (??), evaluating a grid of points for plotting and exploration of the posterior surface, or trying random parameter sets to investigate local minima. Getting ADMB to evaluate these parameter sets is as simple as writing them to the .psv file and then executing ADMB with the option -mceval. See section (2.3) for details on how to do this.

3.3 Output files

3.3.1 Meta data: The hst file

3.3.2 Parameter draws: The psv file

During the mcmc phase, saved parameter values, in bounded space, are written to a binary file called <model name>.psv. This file can be read into R using the following commands:

The first element in the .psv file is the number of active parameters in the model, which then tells R how to parse the following elements into parameter values. Note that the value of *Nout* in nparams*Nout depends on Nmcmc and mcsave and must be specified manually. This is the main file that was designed to be used to extract MCMC draws from ADMB. However, this file only contains parameter values and not derived quantities or other quantities of interest (e.g. MSY or biomass trajectories) which often are of interest.

3.3.3 Derived quantity draws

A simple way of extracting this information is to bypass the psv file altogether and use a C++ function to write a .csv file containing whatever elements are desired. This can be accomplished inside the ADMB .tpl file with just a few lines of code. Inside the DATA_SECTION section use the following code to create an IO object that writes values to a .csv file, similar to the function cout which prints to screen.

```
!!CLASS ofstream MCMCreport("MCMCreport.csv",ios::app);
```

Then, inside the PROCEDURE_SECTION the function can be used to write both parameters, derived quantities, or other information about the model.

```
if(mceval_phase()){
   if(header==1) {
       MCMCreport << "a,b,NLL,ab" << endl;
       header=0;
   }
   MCMCreport << a <<"," << b << "," << NLL << "," << ab << endl;
}</pre>
```

The MCMCreport object is used just like cout and is executed only during the mceval phase so that only saved values are written to the file. Naturally this code can be used anywhere in the procedure section, and this may be a useful diagnostic tool in some situations. New draws are appended to the MCMCreport.csv file so that it must be deleted in between MCMC runs.

3.4 Restarting a chain

Peter: todo

3.5 Convergence diagnostics

Burn-in and thinning, how to check this? What happens if not independent?

3.6 Starting values and scaling

Where the algorithm starts from (MLE) and the scaling process (default and user options). Must discard these draws!

3.7 Metropolis-Hastings

The default MCMC algorithm used by ADMB is the Metropolis-Hastings (MH) algorithm. This algorithm has been around for decades, is simple to implement and used widely.

This algorithm will be most efficient when the posterior surface mimics a multivariate Normal distribution.

3.7.1 Algorithm

Let

f= the ADMB objective function c= an unknown normalization constant Xcur= current parameter vector Xprop= a proposed parameter vector U= a randomly drawn uniform value in [0,1]

Then

$$Xnew = \begin{cases} Xprop & \text{if } U \leq \frac{cf(Xprop)}{cf(Xcur)} \\ Xcur & \text{otherwise} \end{cases}$$
 (1)

The proposal (or "jump") function proposes new parameter vectors given the current set. The default behavior for ADMB is to use a multivariate normal distribution centered at the current vector:

$$Xprop \sim MVN(Xcur, \Sigma)$$

where Σ is the covariance matrix obtained by inverting the Hessian at the posterior mode. In ADMB there are options to modify the proposal function to achieve better efficiency.

3.7.2 MCMC Arguments

-mcmc N	Run N MCMC iterations
-mcsave N	Save every N th MCMC iterations
-mcscale N	Rescale step size for first N iterations

Table 1: ADMB runtime arguments for Metropolis-Hastings MCMC

3.7.3 mcprobe

3.7.4 mcrb

The -mcrb N option (which stands for rescaled bounded) alters the covariance matrix used to propose new parameter sets in the MH algorithm. Its intended use is to create a more efficient MCMC sampler so the analyses run faster.

The option will be most effective under circumstances where the correlation between parameters at the MPD is higher than other regions of the parameter space. In this case, the algorithm may make efficient proposals at the MPD, but inefficient proposals in other parts of the space. By reducing the correlation using mcrb the proposal function may be more efficient on average across the entire parameter space and require less thinning.

¹Technically a bounded multivariate normal

The mcrb option is a set of calculations performed on the original correlation matrix, as follows.

$$\begin{split} & \boldsymbol{\Sigma}_{\text{old}} = \begin{bmatrix} 1 & \cdots & \rho_{1,n} \\ \vdots & \ddots & \vdots \\ \rho_{n,1} & \cdots & 1 \end{bmatrix} & \text{The original correlation matrix} \\ & \boldsymbol{L} = \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ L_{n,1} & \cdots & L_{n,n} \end{bmatrix} & \text{Lower Choleski decomposition of } \boldsymbol{\Sigma}_{\text{old}} \\ & \boldsymbol{\hat{L}} = \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ L_{n,1}^{N/10} & \cdots & L_{n,n}^{N/10} \end{bmatrix} & \text{Raise elements to power user supplied } N \\ & \boldsymbol{\tilde{L}} = \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ \frac{\hat{L}_{n,1}}{|\hat{L}_{n,\cdot}|} & \cdots & \frac{\hat{L}_{n,n}}{|\hat{L}_{n,\cdot}|} \end{bmatrix} & \text{Normalize rows of } \hat{L} \end{split}$$

 $\Sigma_{\rm rb} = \tilde{\mathbf{L}}\tilde{\mathbf{L}}^T$ Calculate new correlation matrix

By working with the Choleski decomposition of the correlation matrix, the algorithm ensures that the rescaled bounded matrix used in the MCMC remains a valid correlation matrix (i.e. positive definite).

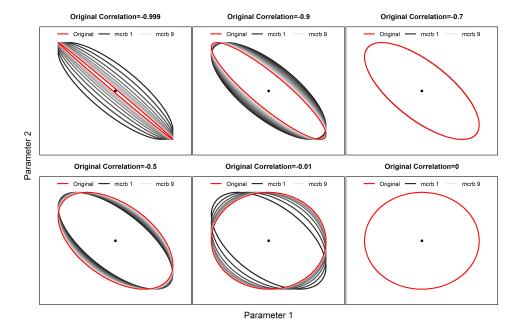


Figure 1: The effect of mcrb on a variety of correlations between two hypothetical parameters. Note that the effect of setting N=9 depends on the original correlation.

3.7.5 Example MCMC

We demonstrate these concepts using the "simple" model packaged with ADMB, which is a contrived two parameter linear model (y = ax + b). First we run the model without any thinning by specifying mcsave=1 (figure 3). The MCMC chain is clearly autocorrelated from the acf plots and the traces (not show). We now rerun the chain with mcsave=100 (figure 3), in effect running 100 times the samples and saving every 100^{th} . This helps reduce the autocorrelation and produces independent draws from the posterior of interest.

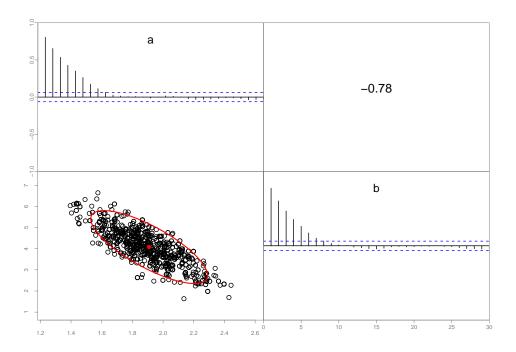


Figure 2: The samples from a simple model with mcsave=1. Note the high autocorrelation of both parameters. The red ellipses show the estimated pairwise parameter covariances, and the red point the MPD.

3.7.6 User-supplied correlation matrix

If the MLE covariance is inefficient at proposing. Why do this? How? Show code for how to do this, and talk about positive definitness.

3.8 Hyrbid

The "hybrid" option in ADMB is an implementation of an MCMC algorithm based on Hamiltonian dynamics. Here we provid a simplified overview ² of the algorithm, with the aim of providing users an intuition about its behavior and properties and how to use it within ADMB. This section is based on [1], which provides a thorough review of the algorithm, including background motivation, proof of ergodicity, and illustrative examples³.

The hybrid method is different from the MH algorithm in how it proposes new parameter values. Instead of proposing random states based on the current value, the hybrid method uses derivatives to follow a contour of the posterior surface. By doing so, it (in theory) only proposes states that are very likely to be accepted, and as such will have less autocorrelation.

In practice, a well tuned hybrid chain will need less thinning, if any at all, and run faster. The downside of the algorithm is that it is more difficult to tune than the MH algorithm.

3.8.1 Algorithm

The algorithm utilizes the properties of a physical system known as Hamiltonian dynamics. Hamiltonian dynamics, while based in physics, provides some extremely useful mathematical properties for Bayesian integration via MCMC.

A Hamiltonian system consists of two parameter vectors of equal length: "position" (\mathbf{q}) and "momentum" (\mathbf{p}). How these parameters change over time is described by the Hamiltonian function, $H(\mathbf{q}, \mathbf{p})$. This system

²Ignoring, for example, the transformation of the parameter space via the Choleski decomposition used by ADMB

³This chapter is available at http://www.admb-project.org/developers/workshop/la-jolla-2010/ham-mcmc.pdf/view

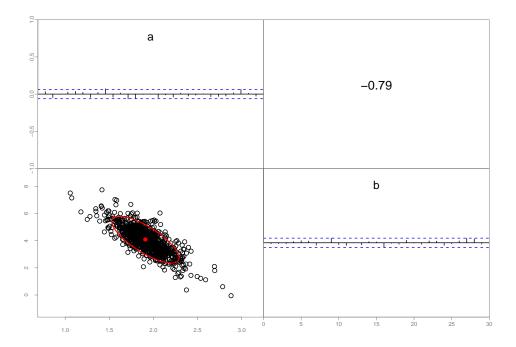


Figure 3: The samples from a simple model with mcsave=100. Note the negligible autocorrelation of both parameters. The red ellipses show the estimated pairwise parameter covariances, and the red point the MPD.

can be conceptualized as a frictionless surface about which an object moves. At some time t an object has a certain height (position) and momentum. The height of the surface is equal to the objective function of our model, and the momentum variables are introduced parameters to ensure the Hamiltonian dynamics are met. Samples from a posterior are generated by simulating the object moving about the joint surface through time, governed by H.

For use with MCMC, H is assumed to be $H(\mathbf{q}, \mathbf{p}) = U(\mathbf{q}) + K(\mathbf{p})$, where U is analogous to the potential energy and K kinetic energy. U is set equal to the ADMB objective function (i.e. the negative log of the posterior density) and K to a diagonal multivariate normal distribution. The hybrid MCMC algorithm samples from the joint posterior, H, but we are only interested in the posterior for U, so K is not saved by ADMB.

The time trajectory of the object through the joint probability space, H, is used to generate proposed parameter sets. Given the form for H above, the fundamental equations of motion are:

$$\frac{dq_i}{dt} = \frac{\partial K}{\partial p_i} \tag{2}$$

$$\frac{dq_i}{dt} = \frac{\partial K}{\partial p_i}$$

$$\frac{dp_i}{dt} = -\frac{\partial U}{\partial q_i}$$
(2)

ADMB uses the "leapfrog" method to discretize equations (2). The leapfrog method is more reliable than the well-known Euler method. It has two tuning parameters: the number of steps to take (hynstep), and the step size ϵ (hyeps). The following sequence of calculations shows a single iteration of the leapfrog method, for the ith variable, and is repeated hynstep times sequentially.

$$\begin{aligned} p_i(t+\epsilon/2) &= p_i(t) - (\epsilon/2) \frac{\partial U}{\partial q_i} q(t) \\ q_i(t+\epsilon) &= q_i(t) + \epsilon \frac{p_i(t+\epsilon/2)}{mi} \\ p_i(t+\epsilon) &= p_i(t+\epsilon/2) - (\epsilon/2) \frac{\partial U}{\partial q_i} q(t+\epsilon) \end{aligned}$$

The leapfrog algorithm moves deterministically through the joint surface along a contour of (appoximately) constant H. That is, for a given starting value of (q_0, p_0) and tuning parameters the trajectory will always end in the same place. Examples of trajectories under different tuning parameters for the leapfrog method are given in figure 4. Note that ADMB calculates the partial derivatives $\frac{\partial U}{\partial q_i}$ at each function evaluation using automatic differentiation. Thus these are available for any model and do not have to be determined analytically, which can be difficult or impossible for large, non-linear models.

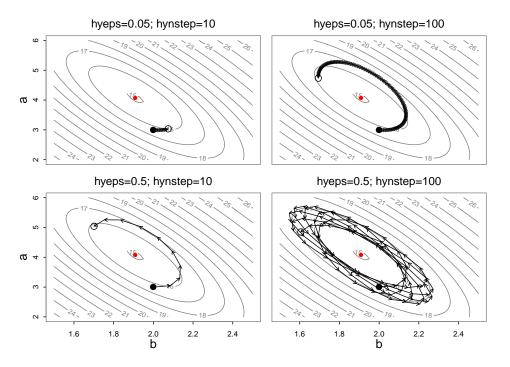


Figure 4: Leapfrog trajectories for different sets of tuning parameters. The posterior surface is shown as contours, and the posterior mode as a red point. The filled black point is the starting point, and the arrows show the trajectory of the leapfrog steps, ending at the open circle representing the proposed set of parameters.

Casting a posterior into a Hamiltonian system and discretizing it with the leapfrog method is simply a way to generate proposed sets of parameters in the larger, stochastic MCMC algorithm. A single iteration of the hybrid MCMC algorithm, as implemented in ADMB, has three steps:

- 1. Propose new momentum variables. New momentum values, p^* are generated from a normal distribution based on the estimated covariance matrix, and independent of the current position variables.
- 2. Propose new position variables. Given the current state of the system, (q, p^*) , new position variables q^* are generated with the leapfrog algorithm using hynstep ⁴ steps and a step size of hyeps.
- 3. Accept or reject the new state. The new state is then updated with a Metropolis step (i.e. accepted or rejected) in the same way as above. Acceptance is expected to be high because the proposed values (q^*, p^*) are rarely into regions of low density for a well tuned chain.

A perhaps intuitive question might be: why bother with the momentum variables at all? One issue is that without the momentum variables, and the Hamiltonian dynamics in general, we would need to account for changes in volume in the acceptance probability (step 3 above)[1]. This would require computing the determinant of the Jacobian matrix of the mapping defined by the dynamics. This Jacobian is not readily available and is often computationally intensive. Thus the need to adopt the Hamilton dynamics framework. Hamiltonian dynamics also provides other properties required for an ergodic Markov chain [1].

⁴Actually a random integers is generated around this value

The hybrid MCMC thus samples from the joint posterior of the position and momentum vectors, but ADMB discards the momentum variables and returns only the position variables. The user can then do inference on those samples in the same was as the Metropolis-Hastings method, given they come from a properly converged (stationary) chain.

3.8.2 Arguments

Arguments for the hybrid algorithm are in general similar to those above, so we only discuss the differences. The main arguments are:

-mcmc N	Run N MCMC iterations
-hybrid	Use the hybrid method
-hynstep N	Mean number of steps for the leapfrog method
-hyeps X	The stepsize for the leapfrog method [X numeric and > 0]

Table 2: ADMB runtime arguments for the hybrid MCMC

Since the estimated covariance matrix is used in the algorithm, the mcdiag, mcrb N, and mcmult options above are also available. The mcprobe argument is not currently supported for the hybrid algorithm.

Note that mcsave N is not an argument for the hybrid and will be ignored. Each MCMC iteration of the hybrid algorithm is saved, such that the user may need to thin the chain manually after running.

3.8.3 Tuning the hybrid algorithm

A tuned hybrid MCMC algorithm often provides a more efficient (computationally) chain than the random walk behavior of the Metropolis-Hastings algorithm. However, the hybrid algorithm is often much more difficult to tune. A thorough review of tuning techniques is beyond the scope of this guide, and we refer users to [1] for further reading of more advanced tuning techniques and intuition about reasonable values⁵.

In most practical applications the hybrid method is tuned via trial and error. That is, values for hynstep and hyeps are tried on a short chain, and the output diagnosed. ADMB uses default values of 0.1 and 10, respectively, and these may be good starting values for most problems. The end goal is to find a set of tuning parameters that produces a well mixing chain with the fewest leapfrog steps. Figure 5 shows the autocorrelation of a parameter from the simple model across different tuning parameters. Note that the top right and bottom left panels show very similar ACF patterns, which should not be a surprise when compared to the corresponding leapfrog trajectories in 4. Further, from that figure we can see that a chain with a hynstep of 100 cycles the surface many times, and although it mixes well, this value could probably be lowered and the runtime reduced without affecting mixing. This is somewhat analagous to having a higher thinning rate than is necessary.

A word of caution regarding the tuning of hybrid chains. For most values of hyeps the leapfrog trajectories will be "stable" in that they will cycle around a contour of H (this can be seen in the last panel in figure 4). However, for values of hyeps that are too large, the method becomes unstable and trajectories diverge (H is no longer constant), causing the algorithm to propose parameters with low density which are then rejected. Unfortunately for real problems, the value of hyeps that is "too big" can vary across the posterior space. Another issue that can arise is that certain combinations of tuning parameters can lead to near periodicity. That is, the leapfrog trajectory ends very near to where it began, after one or more steps. In pathological cases it could cycle forever and never be able to sample regions of the posterior space (i.e. not be ergodic). In practice near periodicity will make for a very slow mixing chain. ADMB mitigates this possibility by randomly drawing the number of leapfrog steps at each MCMC iteration. However, the user should still be aware of these potential issues and be vigilant in diagnosing the mixing behavior of a hybrid chain. Samples from an MCMC chain that is not in equilibrium, or has other issues, can lead to incorrect inference.

 $^{^5}$ The ADMB algorithm works in the transformed space, via the Cholesky decomposition of the estimated covariance matrix, making intuition about tuning even more difficult

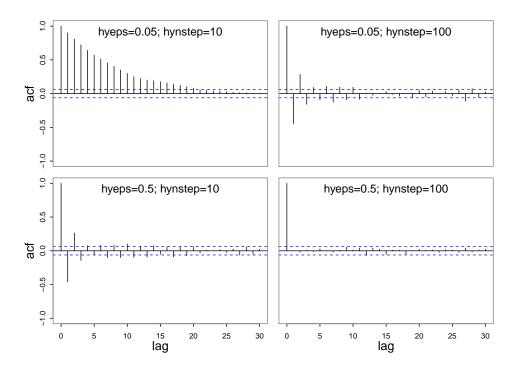


Figure 5: The autocorrelation of the parameter a from the simple model across different tuning parameters of the hybrid method.

References

[1] Steve Brooks, Andrew Gelman, Galin Jones, and Xiao-Li Meng. *Handbook of Markov Chain Monte Carlo*. CRC Press, 2011.