Cosmological Markov Chain Monte Carlo simulation with cmbeasy

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We introduce a Markov Chain Monte Carlo simulation and data analysis package for the cosmological computation package CMBEASY. We have taken special care in implementing an adaptive step algorithm for the Markov Chain Monte Carlo in order to improve convergence. Data analysis routines are provided which allow to test models of the Universe against up-to-date measurements of the Cosmic Microwave Background, Supernovae Ia and Large Scale Structure. The observational data is provided with the software for convenient usage. The package is publicly available as part of the CMBEASY software at www.cmbeasy.org.

1 Introduction

The wealth of recent precision measurements in cosmology places stringent constraints on any model of the Universe. Typically, such a model is given in terms of a number of cosmological parameters. Numerical tools, such as CMBFAST, CAMB, and CMBEASY, permit to calculate the prediction of a given model for the observational data. While these tools are comparatively fast, scanning the parameter space for the most likely model and confidence regions can become a matter of time and computing power. The cost of evaluating models on an n-dimensional grid in parameter space increases exponentially with the number of parameters. In contrast, the Markov Chain Monte Carlo (MCMC) method scales roughly linearly with the number of parameters. The MCMC method has already been used to constrain various models. A popular tool for setting up MCMC simulations is the COSMO-Mc package for the CAMB code, an improved proposal distribution for the local Metropolis algorithm has been proposed in.

We introduce the AnalyzeThis package for CMBEASY. It includes a parallel MCMC driver, as well as routines to calculate the likelihood of a model with respect to various data sets. We took special care in designing a step-proposal strategy that leads to fast convergence.

*It is part of the cmbeasy v2.0 release.
Figure 1: The graphical user interface of CMBEASY. It can be used to marginalize, visualize and print the one and two dimensional likelihoods from the MCMC chains. Shown is the marginalized likelihood in the $\Omega_m h^2 - \Omega_b h^2$ plane of a $\Lambda$CDM model.

and mixing of the chains. The automated step optimization considerably improves performance and is rather convenient. The raw data files can be processed from within a graphical user interface (gui). Using the gui, one can marginalize, visualize and print one and two dimensional likelihood surfaces (see figure 1).

2 Markov Chain Monte Carlo simulation

In the following, we will assume the reader is familiar with the basic ideas of Markov Chain Monte Carlo simulation\textsuperscript{28} and the Metropolis algorithm\textsuperscript{29}. We will now describe our implementation as contained in the released version\textsuperscript{27}.

The global Metropolis algorithm chooses new steps for a Markov Chain via a symmetric proposal distribution $q(\theta_{i-1}, \theta_i) = q(\theta_i, \theta_{i-1})$, where $\theta_i$ is a parameter vector that specifies a given model. In our implementation, we assume flat priors $P(\theta)$ on the parameters, and we assign likelihood zero to any parameter set that has at least one point outside the prior.

A very important aspect of MCMC is to test when the chains are sampling from the underlying distribution. Since at the beginning, the chain migrates from its random starting point to regions of higher likelihood, there is a “burn-in” associated with each chain that must be eliminated prior to parameter estimation. In principle, it may be difficult to tell from a single chain if it has converged. In MCMC, one therefore uses several chains with random starting points and monitors mixing and convergence. Our implementation employs the convergence test of Gelman and Rubin\textsuperscript{10}. The key ingredient for this test is a parameter $R$ which can be
computed from previous chain points. This parameter is a comparison of the variance within the chains compared to the variance between different chains. A value of $R < 1.2$ for each parameter indicates the chains have converged and all previous points should be removed. If one uses the gui for chain analysis, the burn-in is automatically removed.

Since there is no generally accepted procedure to determine when one has generated enough chain points for reliable estimation, the algorithm just runs indefinitely in our implementation. However, any “breaking-criterion” may be implemented easily. The chains may be monitored with external programs during the run.

The number of steps needed for good convergence and mixing depends strongly on the step proposal distribution. If the proposed steps are too large, the algorithm will frequently reject steps, giving slow convergence of the chain. If, on the other hand, the proposed steps are too small, it will take a long time for the chain to explore the likelihood surface, resulting in slow mixing. In the ideal case the proposal distribution should be as close to the posterior distribution as possible – which unfortunately is not known a priori. While a simple Gaussian proposal distribution with step sizes $\sigma$ is sufficient, it is not optimal in terms of computing costs if cosmological parameters are degenerate. Instead of using a naive Gaussian proposal distribution, we sample from a multivariate Gaussian distribution with covariance matrix estimated from the previous points in the chains. By taking into account the covariances among the parameters, we effectively approximate the likelihood contour in extent and orientation – the Gaussian samples are taken along the principal axis of the likelihood contour.

The convergence can be further improved by scaling the covariance matrix with a variable factor $\alpha$. Using $\alpha$, we can cope better in situations where the projected likelihood takes on banana shapes such as in. It also improves the convergence during the early stages when the low number of points available limits the estimate of the covariance matrix. We dynamically increase $\alpha$ if a chain takes steps too often, while we decrease $\alpha$ if the acceptance rate is too low. By this procedure the convergence is speeded up by a factor of about four compared to naive Gaussian sampling.

One can show that modifying the proposal distribution based on previous chain data during the run may lead to a wrong stationary distribution. Therefore, we only apply the dynamical strategy of finding an optimal step proposal during the early stages of the simulation. When the convergence is better than $R = 1.2$ and the chain has calculated a certain number of points, we freeze in the step proposal distribution.

### 3 The Software

The package is part of CMBEASY and consists of two main components. The first one is a MCMC driver using LAM/MPI for parallel execution of each chain. The second one is the `AnalyzeThis` class which is designed to evaluate the likelihood of a given model with respect to various data sets. These sets include the latest data of WMAP TT and TE, ACBAR, CBI, VSA, 2dFGRS, SDSS, the SNe Ia compilations of Riess et al., Tonry et al, and Knop et. al, as well as the IfA Deep Survey SNe Ia data. Data files for all experiments are included for convenience. New data sets are added continuously to the code.

The example MCMC driver consists of two routines: `master()` and `slave()`. Using LAM/MPI for parallel computing, one master and up to ten slaves may be started. The `master()` will determine the initial random starting position for each chain. In a never ending loop, it then sends the parameters to the `slave()`’s and collects the results when the computation is finished. Whenever a step has been successful, it stores the parameters and likelihoods of the last step together with the number of times the chain remained at the same point in parameter space in a new line of one file per chain. The `master()` monitors convergence and mixing and determines the next step for the `slave()`. Before freeze in, the covariance is estimated and the step proposal
accordingly modified. After freeze in, the proposal distribution remains unchanged.

The gui may be used to process the raw output files of the MCMC chains. It enables quick and convenient analysis of MCMC simulations. To get started immediately, we include raw data from an example MCMC run in the resources directory of cmbeasy. Two and one dimensional marginalized likelihoods may then be plotted and printed from within the gui (see figure 1).

4 Conclusions

We have introduced the AnalyzeThis package, which can be used to constrain cosmological models using observational data sets. The AnalyzeThis class provides many functions to compute the likelihood of a model with respect to measurements of the CMB, SNe Ia and Large Scale Structure.

In order to constrain models of the Universe with a substantial number of parameters, we include a Markov Chain Monte Carlo driver. As the MCMC step strategy determines the convergence speed of the chains, we implemented a multivariate Gaussian sampler with an additional dynamical scaling.

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