evolMC: a package for Monte-Carlo simulation

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Abstract

Sampling from multi-modal target distributions proves difficult for basic MCMC methods. Borrowing from the evolutionary based algorithms of optimization theory, Liang and Wong [2000] introduced evolutionary Monte Carlo (EMC). EMC begins with parallel tempering and then adds to it a step in which sequences intelligently evolve by learning from each other. A comparative simulation highlights the effectiveness of EMC over other sampling methods.

Markov Chain Monte Carlo methods, as exemplified by the classic Metropolis *et al.* [1953] and Hastings [1970] algorithms, are an important tool in contemporary statistics. However, the basic algorithms often do not work well in situations where the distribution of interest possesses multiple modes. Several extensions have been suggested to alleviate this problem. In this paper we explore two such algorithms, Parallel Tempering [Swendsen and Wang,

1986], and a further extension, the Evolutionary algorithms of Liang and Wong [2000].

Parallel tempering simulates multiple sequences from a "heated" target distribution, and then proposes to exchange information between the chains according to the Metropolis rule. This helps to encourage a more thorough global search of the support space. [Liang *et al.*, 2011] Evolutionary Monte Carlo (EMC) builds upon parallel tempering by blending with it ideas taken from evolutionary biology. In particular, the Chromosomal crossovers that are observed in Meiosis are simulated. Such crossovers are thought to be an important component of the success of sexual reproduction.

Iterations of the EMC algorithm consist of three operations: mutation, crossover, and exchange. Each type of operation makes a specific type of modification to the current population, and the change is carried forward to the next generation with a probability governed by a Metropolis-type rule.[Liang *et al.*, 2011]

In general terms, a mutation operation adds noise to the current population. This can be analogous to a basic random walk type proposal, but more elaborate methods have been proposed. A crossover operator consists of randomly selecting two individuals and generating replacement individuals by somehow mixing the parent values, analogous to the Chromosomal crossovers that sometimes occur during Meiosis. An exchange step proposes a switch of two randomly selected individuals without switching their associated temperatures.

In the remainder of this paper we compare the performance of the EMC algorithm to parallel tempering and a naïve Metropolis sampler in the context of a 3 dimensional distribution with 20 modes. Section two describes in greater detail the algorithms used and the simulation setup. While results of the simulation are presented and discussed in sections 3 and 4.

2 Methods

The target distribution for our study is a 20-part mixture of trivariate Gaussian distributions. Each part of the mixture is $\mathcal{N}_3(\mu_i, 0.1I_3)$, and each vector μ_i is located uniformly in $[-10, 10] \times [-10, 10] \times [-10, 10]$. This distribution possesses numerous modes that are separated by relatively large regions of low probability, making it challenging for a basic Metropolis sampler to mix between the modes.

2.1 Algorithms

The discussion of population based Monte Carlo methods necessarily begins by introducing some terminology. The following recounts the terminology given in Chapter 5 of Liang *et al.* [2011]: We wish to sample from a distribution $f(x|t) \propto \exp\{-H(x)/t\}$, where $t \geq 1$ is called the *temperature* and $H(x)$, called the *fitness function*, corresponds to the negative log-density of x, up to a constant. A *population* $\mathbf{x}$ consists of N *individuals* x_i, $i = 1, \ldots, N$, and we also define an associated set of temperatures $\mathbf{t} = (t_1, \ldots, t_N)$. ($x_i \in \mathbb{R}^d$ and

the t_i are in descending order.) Each individual x_i is independently sampled from the distribution $f_i(x_i) \propto f(x_i|t_i)$. For any such distribution, the *partition function* $Z(t) = \int_{\mathcal{X}} f(x|t)dx$ is the inverse of the normalizing constant. The *Boltzmann distribution* of the population $\mathbf{x}$ is the product of the individual distributions, $f(\mathbf{x}) \propto \exp\{-\sum_{i=1}^{N} H(x_i)/t_i\}$, with $Z(\mathbf{t}) := \prod_{i=1}^{N} Z(t_i)$ as the inverse of the normalizing constant.

The EMC algorithm we have implemented is described briefly in Algorithms 1–4. The mutate step uses a simple random-walk approach, where the variance of the noise distribution depends on the temperature of the individual being modified. The crossover we used is a simple single-splice version, where the parents are selected with weights based on their fitness.

2.2 Simulations

The algorithms described have several tuning parameters that the user must supply. We ran simulations in an attempt to come to a qualitative understanding of the effects that these tuning parameters have on the performance of the Markov Chain. We ran chains on all combinations of options described below.

The choice of mutator distribution: Gaussian noise with variance dependent on the temperature, or a uniform proposal with no temperature dependance. We tested three different temperature ladders: $(1, 5)$, $(1, 2, 4, 8, 15)$, and $(1, 5, 15, 30, 50)$. (There is a great deal of freedom in the selection of the temperature ladder, but we attempted to study the effect of an insuffi-

cient number of temperature settings, as well as the effect of changing the spacing of temperature levels.) The mutation/crossover selection probabilities: $p_m \in \{0.1, 0.5, 0.9, 1.0\}$. Note that $p_m = 1.0$ is equivalent to parallel tempering.

The chains were run for a $20,000$ iterations. This is not nearly a long enough run to accurately estimate the mixing proportions, however it should allow us to get a sense of how easily the chains explore the space. If a mode is not explored by this point, then the chain is clearly mixing quite poorly. However if all modes are being visited in this amount of time then the average dwelling time per mode is at most approximately 1000 iterations, which is not a shockingly large number.

3 Results

3.1 Software

We present the R package evolMC, which is a framework for doing Markov-Chain Monte Carlo simulations. The evolMC package includes implementations of several MCMC algorithms, including Metropolis-Hastings, Gibbs, parallel tempering, and the evolutionary updating methods. The package is available from `http://github.com/grady/evol-mc/`.

The package aims to provide a general framework for constructing a chain, leaving it up to the user to provide the pieces specific to the problem. The user must first define a *state object* and then implement a number of functions

which act on this state object. In many traditional cases this state object can simply be a vector of reals, but any R object (e.g. a phylogenetic tree object defined by a 3rd-party package) can be used. This generality departs from many existing R MCMC packages, which enforce vector- or array-type structures for the random elements in question.

The functions provided by evolMC will eventually produce a *chain* object, which is simply an R list where each element is an instance of the state object. A function is provided to convert this object into a `coda::mcmc.list` object. The evolMC package includes a vignette demonstrating a few basic use cases, with example code.

The main job of the user of evolMC is to define a few basic functions which can interact in specified ways with whatever object is selected to represent states of the chain. For example, the user will often need to implement a function which evaluates a log-density for a given state. Using the routines provided by evolMC, one will then manipulate these functions, eventually producing a function which implements some desired MCMC algorithm.

3.2 Simulations

In the simulations discussed in the previous section, the best criterion to assess the various methods and tuning parameters was the number of modes the chain was able to sample from. Figure 1 contains a plot of the states observed in select situations. The points are layered so that chains that found more modes are behind those which found only a few modes. Table 1

displays a count of the modes found for a subset of the scenarios tested.

In terms of methods, the multivariate sampler generally only finds a single mode. Parallel tempering and evolutionary Monte Carlo were comparable, depending on the tuning parameters. More temperatures being included in the temperature ladder led to more modes being sampled from, as chains were more easily able to move around the entire space. In addition, using the Gaussian proposal with a variance weighted by the temperature for the mutation operation produced better results than using a uniform proposal with fixed support.

The most surprising and informative result concerns the probability of mutation or crossover (the additional operation introduced in the evolutionary MC method). Lower probabilities for the crossover operation (and therefore higher probabilities for the mutation operation) resulted in more modes of the target distribution being sampled from. In fact, for this problem parallel tempering produced samples just as good or better than the evolutionary Monte Carlo method did.

4 Discussion

Evolutionary Monte Carlo adds an additional operation, crossover, onto the parallel tempering algorithm, which Liang *et al.* [2011] claims allows EMC to more fully explore the target distribution's space. However, our findings in this situation are at odds to those of Liang's.

In almost all five-tuple temperature scenarios, both EMC and parallel tempering were able to find almost every mode; the exceptions to this rule all employed the uniform mutation proposals. However, the remainder of our simulations clearly show that for this target distribution parallel tempering is sufficient to fully explore the sample space, provided a suitable temperature ladder is chosen. The crossover operation does not appear to significantly improve the mixing of the chain.

The crossover that we implemented for this simulation study is perhaps the simplest example of a crossover procedure, and indeed Liang *et al.* [2011] suggests a few more complicated ones. Further work is warranted to explore the performance of these more complicated crossover options. The problem of automated temperature selection is also discussed, and implementation of these methods is a next step in improving the usability of `evolMC`.

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A evolMC

The evolMC package includes a vignette demonstrating a few basic use cases, with example code. Here we briefly discuss the architectural vision underlying the package and a few of the most important functions.

evolMC was designed to be as flexible as possible, and hence it operates on a quite abstract level. It is written in a very functional style of programming; most of the important functions in evolMC accept functions as arguments and return new functions. An important goal was for the user to be free to use whatever object they wish to represent a realization of the random element in question. This departs from many existing R MCMC packages, which require vector- or array-type structures for the random elements in question.

The main job of the user of evolMC is to define a few basic functions which

can interact in specified ways with whatever object is selected to represent states of the chain. For example, the user will often need to implement a function which evaluates a log-density for a given state. Using the routines provided by evolMC, one will then manipulate these functions, eventually producing a function which implements some desired MCMC algorithm.

The core function in evolMC is `iterate(n,f,x)`. This function is also among the least interesting, because it simply creates a list where the $(k+1)$-th element is $f^k(x)$. (Function exponentiation means iterated application here.) If the provided function `f` is "carefully selected" then the resulting chain might have "desirable properties". Of course, we are likely interested in the case where the desirable property in question is that the resulting list represents a sample from some target distribution. Most other functions in the package exist to help one in constructing a function `f` with specific desirable properties.

Perhaps the most basic MCMC algorithm is the Gibbs sampler. Suppose we want to sample from $[x, y]$. If we can sample from $[x|y]$ and $[y|x]$, then we can implement a Gibbs sampler. To do this one need only implement functions `rxy` and `ryx`, which do the respective sampling. These functions should accept the current state as their first argument, and return a new state object with the relavant changes made.

Once one has these functions, the gibbs function can be used to produce a new updating function which will implement the Gibbs algorithm. The basic signature is `gibbs(...)`. The ... argument allows one to provide any number

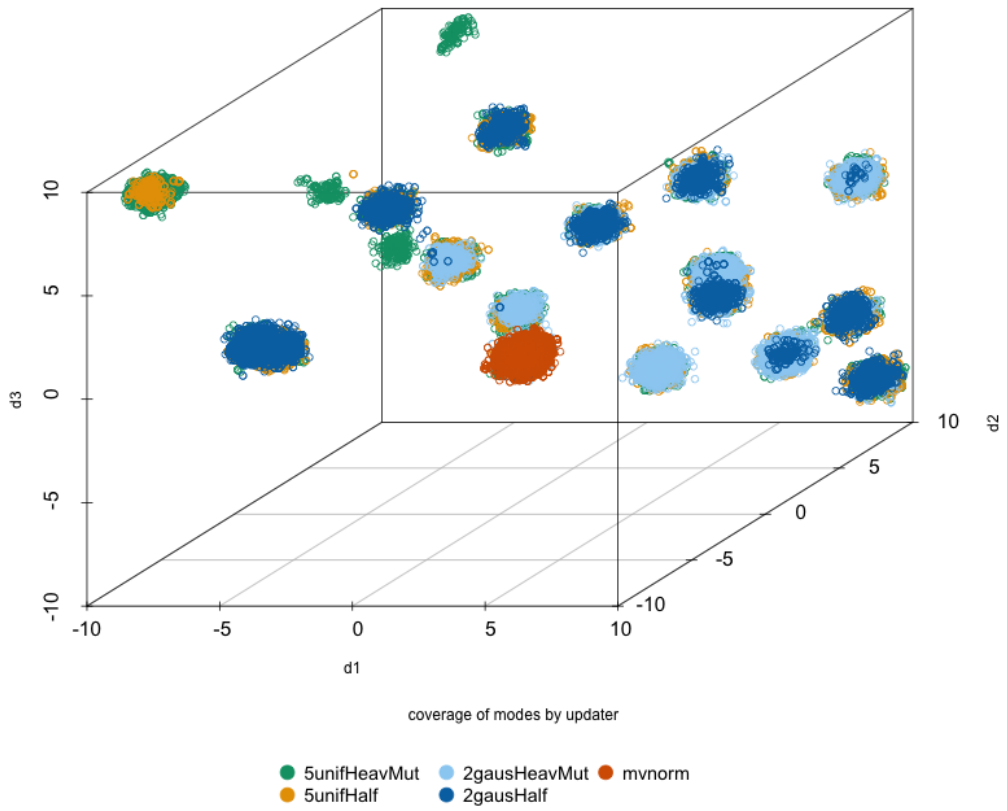
of updating functions; in our case we have two, `rxy` and `ryx`. The result of `gibbs(rxy,ryx)` is a new "carefully selected" function with signature `function(state)` which acts as a Gibbs updater. If called repeatedly (e.g. by iterate) it will alternate between using `rxy` and `ryx` to update the state.[1]

A second important algorithm is the Metropolis algorithm. The function `metropolis` helps one to construct an updating function which implements Metropolis-Hastings. To use this function one must first implement: the log-density function for the target distribution (`ln.d`); a proposal generator function (`r.prop`); and (if required) a log-density function for the proposal generator (`ln.d.prop`). A call `metropolis(ln.d, r.prop, ln.d.prop)` will return a "carefully selected" function (with signature `function(state)`), which implements the Metropolis-Hastings scheme you have defined.

These three basic building blocks can be used to construct a surprising number of more advanced MCMC algorithms, and indeed many of the more advanced algorithms provided by evolMC are constructed using only these pieces.

[1]The sequential choice of updating functions is the default mode of operation for the function returned by `gibbs`. It can also stochastically select an updating function according to provided weights.

Figure 1: Scatterplot of states realized by selected tuning parameter settings.



Temps	Mutator	p_m	Modes
two	Gaussian	0.1	2
two	Gaussian	0.9	12
two	Gaussian	0.5	13
two	Gaussian	1	14
five.wide	Gaussian	0.1	17
five	Gaussian	0.1	18
five	Gaussian	0.5	20
five.wide	Gaussian	0.5	20
five	Gaussian	0.9	20
five.wide	Gaussian	0.9	20
five	Gaussian	1	20
five.wide	Gaussian	1	20

Table 1: Number of modes discovered by the chain for selected tuning parameter combinations.

Algorithm 1 Evolutionary Monte Carlo

procedure EMC
  with prob p_m ▷ p_m is the *mutation probability*.
    MUTATE
  otherwise
    CROSSOVER
  end w/prob
  EXCHANGE
end procedure

Algorithm 2 A random-walk *mutation*.

procedure MUTATE
  Copy the current population to x.
  for all individuals in x **do**
    $y \leftarrow \mathcal{N}_d(x_i, t_i\sigma^2 I)$
    with prob $\min\{1, \exp(\cdots)\}$
      $x_i \leftarrow y$
    end w/prob
  end for
  Set current population to x.
end procedure

Algorithm 3 The fitness-weighted *crossover*.

procedure CROSSOVER
  Copy the current population to x.
  for all individuals in x **do**
    $w_i \leftarrow \exp(-H(x_i))$
  end for
  Select k uniformly from $\{1\colon d\}$.
  Select i from $\{1\colon N\}$ with weights proportional to $\{w_\cdot\}$.
  Select j uniformly from $\{1\colon N\}\backslash\{i\}$.
  In x, swap elements $k\colon d$ of individuals i and j.
  with prob $\min\{1, \exp(-H(x_i)/t_i + H(x_j)/t_j + \cdots)\}$
    Set the current population to x.
  end w/prob
end procedure

Algorithm 4 The *exchange* attempts to swap individuals between neighboring temperature states.

procedure EXCHANGE
  Copy the current population to x.
  Select i uniformly from $\{1{:}\,N\}$.
  Select j uniformly from $\{i \pm 1\} \cap \{1{:}\,N\}$.
  Swap individuals i, j of x.
  with prob $\min\{1, \exp(-H(x_i)/t_i + H(x_j)/t_j)\}$
    Set the current population to x.
  end w/prob
end procedure