Technical Report No. 2005, Department of Statistics, University of Toronto

Slice Sampling

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29 August 2000

Abstract. Markov chain sampling methods that automatically adapt to characteristics of the distribution being sampled can be constructed by exploiting the principle that one can sample from a distribution by sampling uniformly from the region under the plot of its density function. A Markov chain that converges to this uniform distribution can be constructed by alternating uniform sampling in the vertical direction with uniform sampling from the horizontal 'slice' defined by the current vertical position, or more generally, with some update that leaves the uniform distribution over this slice invariant. Variations on such 'slice sampling' methods are easily implemented for univariate distributions, and can be used to sample from a multivariate distribution by updating each variable in turn. This approach is often easier to implement than Gibbs sampling, and more efficient than simple Metropolis updates, due to the ability of slice sampling to adaptively choose the magnitude of changes made. It is therefore attractive for routine and automated use. Slice sampling methods that update all variables simultaneously are also possible. These methods can adaptively choose the magnitudes of changes made to each variable, based on the local properties of the density function. More ambitiously, such methods could potentially allow the sampling to adapt to dependencies between variables by constructing local quadratic approximations. Another approach is to improve sampling efficiency by suppressing random walks. This can be done using 'overrelaxed' versions of univariate slice sampling procedures, or by using 'reflective' multivariate slice sampling methods, which bounce off the edges of the slice.

Keywords: Markov chain Monte Carlo, adaptive methods, Gibbs sampling, Metropolis algorithm, overrelaxation, dynamical methods.

1 Introduction

Markov chain methods such as Gibbs sampling (Gelfand and Smith 1990) and the Metropolis algorithm (Metropolis, *et al* 1953, Hastings 1970) can be used to sample from many of the complex, multivariate distributions encountered in statistics. However, to implement Gibbs sampling, one may need to devise methods for sampling from non-standard univariate distributions, and to use the Metropolis algorithm, one must find an appropriate 'proposal' distribution that will lead to efficient sampling. The need for such special tailoring limits the routine use of these methods, and inhibits the development of software that automatically constructs Markov chain samplers from model specifications. Furthermore, many common Markov chain samplers are inefficient, due to a combination of two flaws. First, they may try to make changes that are not well adapted to the local properties of the density function, with the result that changes must be made in small steps. Second, these small steps take the form of a random walk, in which about n^2 such steps are needed in order to move a distance that could be traversed in only n steps if these steps moved consistently in one direction.

In this paper, I describe a class of 'slice sampling' methods that can be applied to a wide variety of distributions. Simple forms of univariate slice sampling are an alternative to Gibbs sampling that avoids the need to sample from non-standard distributions. These slice sampling methods can adaptively change the scale of changes made, which makes them easier to tune than Metropolis methods, and also avoids problems that arise when the appropriate scale of changes varys over the distribution. More complex slice sampling methods can adapt to the dependencies between variables, allowing larger changes than would be possible with Gibbs sampling or simple Metropolis methods. Slice sampling methods that improve sampling by suppressing random walks can also be constructed.

Slice sampling originates with the observation that one can sample from a univariate distribution by sampling points uniformly from the region under the curve of its density function, and then looking only at the horizontal coordinates of the sample points. A Markov chain that converges to this uniform distribution can be constructed by alternately sampling uniformly from the vertical interval defined by the density at the current point, and from the union of intervals that constitutes the horizontal 'slice' though the plot of the density function that this vertical position defines. If this last step is still difficult, one may substitute some other update that leaves the uniform distribution over the current slice invariant. To sample from a multivariate distribution, such single-variable slice sampling updates can be applied to each variable in turn. The details of these single-variable slice sampling methods are described in Section 4.

One can also apply the slice sampling approach to a multivariate distribution directly, as described in Section 5, by sampling uniformly under the multidimensional plot of its density function. As for a univariate distribution, this can be done by alternately sampling uniformly from the vertical interval from zero up to the density at the current point, and then uniformly from the slice defined by this vertical position. When the slice is high-dimensional, how to efficiently sample from it is less obvious than for single-variable slice sampling, but one gains the possibility of sampling in a way that respects the dependencies between variables. I show how, in the context of slice sampling, the way changes are proposed can be adapted to respect these dependencies, based on local information about the density function. In particular, local quadratic approximations could be constructed, as have been used very successfully for optimization problems. Adaptive slice sampling appears to be simpler than a somewhat analogous scheme proposed for the Metropolis algorithm (Mira 1998, Chapter 5; Tierney and Mira 1999; Green and Mira 1999). However, further research will be needed to fully exploit the adaptive capabilities of multivariate slice sampling.

One might instead accept that dependencies between variables will lead to the distribution being explored in small steps, but try at least to avoid exploring the distribution by an inefficient random walk, which is what happens when simple forms of the Metropolis algorithm are used. The benefits of random walk suppression are analysed theoretically in some simple contexts by Diaconis, Holmes, and Neal (in press). Large gains in sampling efficiency can be obtained in practice when random walks are suppressed using the Hybrid Monte Carlo or other dynamical methods (Duane, Kennedy, Pendleton, and Roweth 1987; Horowitz 1991; Neal 1994; and for reviews from a more statistical perspective, Neal 1993, 1996), or by using an overrelaxation method (Adler 1981; Barone and Frigessi 1990; Green and Han 1992; Neal 1998). Dynamical and overrelaxation methods are not always easy to apply, however. Use of Markov chain samplers that avoid random walks would be assisted by the development of methods that require less special programming and parameter tuning.

Two approaches to random walk suppression based on slice sampling are discussed in this paper. In Section 6, I show how one can implement an overrelaxed version of the single-variable slice sampling scheme. This may provide the benefits of Adler's (1981) Gaussian overrelaxation method for more general distributions. In Section 7, I describe slice sampling analogues of dynamical methods, which move around a multi-variable slice using a stepping procedure that proceeds consistently in one direction while reflecting off the slice boundaries. Although these more elaborate slice sampling methods require more tuning than the single-variable slice sampling schemes, they may still be easier to apply than alternative methods that avoid random walks.

To illustrate the advantages of the adaptive nature of slice sampling, I show in Section 8 how it can help avoid disaster when sampling from a distribution that is typical of priors for hierarchical Bayesian models. Simple Metropolis methods can give the wrong answer for this problem, while providing little indication that anything is amiss.

This paper concludes (in Section 9) with a discussion of the merits of the various slice sampling methods in comparison with other Markov chain methods, and of their suitability for routine and automated use. Below, I set the stage by discussing general-purpose Markov chain methods that are currently in wide use. Readers who are quite familiar with Markov chain sampling and are eager to get to the main idea can skip immediately to Section 3.

2 General-purpose Markov chain sampling methods

Applications of Markov chain sampling in statistics often involve sampling from many distributions. In Bayesian applications, we must sample from the posterior distribution for the parameters of a model given certain data. Different datasets will produce different posterior distributions, which may differ in important characteristics such as diffuseness and multimodality. Furthermore, we will often wish to consider a variety of models. For routine use of Markov chain methods, it is important to minimize the amount of effort that the data analyst must spend in order to sample from all these distributions. Ideally, a Markov chain sampler would be constructed automatically for each model and dataset.

The Markov chain method most commonly used in statistics is Gibbs sampling, popularized by Gelfand and Smith (1990). Suppose that we wish to sample from a distribution over n state variables (eg, model parameters), written as $x = (x_1, \ldots, x_n)$, with probability density $p(x)$. Gibbs sampling proceeds by sampling in succession from the conditional distributions for each x_i given the current values of the other x_j for $j \neq i$, with conditional densities written as $p(x_i \,|\, \{x_j\}_{j \neq i})$. Repetition of this procedure defines a Markov chain which leaves the desired distribution invariant, and which in many circumstances is ergodic (eg, when $p(x) > 0$ for all x). Running the Gibbs sampler for a sufficiently long time will then produce a sample of values for x from close to the desired distribution, from which the expectations of quantities of interest (eg, posterior means of parameters) can be estimated.

Gibbs sampling can be done only if we know how to sample from all the required conditional distributions. These sometimes have standard forms for which efficient sampling methods have been developed, but there are many models for which sampling from these conditional distributions requires the development of custom algorithms, or is infeasible in practice (eg, for multilayer perceptron networks (Neal 1996)). Note, however, that once methods for sampling from these conditional distributions have been found, no further tuning parameters need be set in order to produce the final Markov chain sampler.

The routine use of Gibbs sampling has been assisted by the development of Adaptive Rejection Sampling (ARS) (Gilks and Wild 1992; Gilks 1992), which can be used to efficiently sample from any conditional distribution whose density function is log concave, given only the ability to compute some function, $f_i(x_i)$, that is proportional to the conditional density, $p(x_i \,|\, \{x_j\}_{j \neq i})$ (the ability to also compute the derivative, $f_i'(x_i)$, is helpful, but not essential). This method has been used for some time by the BUGS software (Thomas, Spiegelhalter, and Gilks 1992) to automatically generate Markov chain samplers from model specifications. The first step in applying ARS is to find points on each side of the mode of the conditional distribution (one of which can be the current point). This will in general require a search, which will in turn require the choice of some length scale for an initial step. However, the burden of setting this scale parameter is lessened by the fact that a good value for it can be chosen 'retrospectively', based on past iterations of the Markov chain, without invalidating the results (since the setting of this parameter affects only the computation time, not the distribution sampled from).

The Adaptive Rejection Metropolis Sampling (ARMS) method (Gilks, Best, and Tan 1995) generalizes ARS to conditional distributions whose density functions may not be log-concave. However, when the density is not log-concave, ARMS does not produce a new point drawn independently from the conditional distribution, but merely updates the current point in a fashion that leaves this distribution invariant. Applying ARMS to sample from the conditional distribution of each variable in succession will result in an equilibrium distribution that is exactly correct, but when some conditional distributions are not log-concave, it may take longer to approach this equilibrium than would be the case if true Gibbs sampling were used. Also, when a conditional distribution is not log-concave, the points used to set up the initial approximation to it must not be chosen with reference to past iterations, as this could result in the wrong distribution being sampled (Gilks, Neal, Best, and Tan 1997). The initial approximation must be chosen based only on prior knowledge (including any preliminary Markov chain sampling runs), and on the current values of the other variables. Unlike ARS, neither the current value of the variable being updated, nor any statistics collected from previous updates (eg, the typical scale of changes) can be used. This hinders routine use of the method.

Another general way of constructing a Markov chain sampler is to perform Metropolis updates (Metropolis, *et al* 1953, Hastings 1970), either for each variable in turn, as with Gibbs sampling, or for all variables simultaneously. A Metropolis update starts with the random selection of a 'candidate' state, drawn from a 'proposal' distribution. The candidate state is then accepted or rejected as the new state of the Markov chain, based on the ratio of the probability densities of the candidate state and the current state. If the candidate state is rejected, the new state is the same as the old state.

A simple 'random-walk' Metropolis scheme can be constructed based on a symmetric proposal distribution (eg, Gaussian) that is centred on the current state. All variables could be updated simultaneously in such a scheme, or alternatively, one variable could be updated at a time. In either case, a scale parameter is required for each variable to fix the width of the proposal distribution in that dimension. For the method to be valid, these scale parameters must not be set on the basis of past iterations, but rather only on the basis of prior knowledge (including preliminary runs), and the current values of variables that are not being changed in the present update. Choosing too large a value for the scale of a proposal distribution will result in a high rejection rate, while choosing too small a value will result in inefficient exploration via a random walk with unnecessarily small steps. Furthermore, the appropriate scale for Metropolis proposals may vary from one part of the distribution to another, in which case no single value will produce acceptable results. Selecting a scale at random from some range can sometimes alleviate these problems, but at a large cost in wasted effort when the scale selected is inappropriate.

It is tempting to tune the Metropolis proposal distribution based on the rejection rate in past iterations of the Markov chain, but such 'retrospective tuning' is not valid in general, since it can disturb the stationary distribution to which the process converges (as was also the case for ARMS). Fixing the proposal distribution based on a preliminary run is allowed, but if the original proposal distribution was not good, such a preliminary run may not have sampled from the whole distribution, and hence may be a bad guide for tuning.

We therefore see that although Gibbs sampling and Metropolis methods have been used to do much useful work, there is a need for better methods, that can be routinely applied in a wider variety of situations. One of my objectives in this paper is to find variations on slice sampling that can be used to sample from any continuous distribution, given only the ability to evaluate a 'black-box' function that is proportional to its density, and in some cases, to also evaluate the gradient of the log of this function. For many distributions, these new methods will not sample more efficiently than true Gibbs sampling or a well-designed Metropolis scheme, but the slice sampling methods will often requiring less effort to implement and tune. For some distributions, however, slice sampling can be much more efficient, because it can adaptively choose a scale for changes appropriate for the region of the distribution currently being sampled. Slice samplers that adapt in more elaborate ways, or that are designed to suppress random walks, can potentially be much faster than simple Metropolis methods or Gibbs sampling.

3 The idea of slice sampling

Suppose we wish to sample from a distribution for a variable, x, taking values in some subset of $\Re^n$, with density function proportional to some function $f(x)$. We can do this by sampling uniformly from the $n+1$ dimensional region that lies under the plot of $f(x)$. This idea can be formalized by introducing an auxiliary real variable, y, and defining a joint distribution over x and y that is uniform over the region $U = \{\, (x,y) \;:\; 0 < y < f(x) \,\}$ below the curve or surface defined by $f(x)$. That is, the joint density for (x,y) is

$$p(x,y) \;\; = \;\; \begin{cases} 1/Z & \text{if } 0 < y < f(x) \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

where $Z = \int f(x)\, dx$. The marginal density for x is then

$$p(x) \;\; = \;\; \int_0^{f(x)} (1/Z)\, dy \;\; = \;\; f(x) \,/\, Z \tag{2}$$

as desired. To sample for x, we can sample jointly for (x,y), and then ignore y.

Generating independent points drawn uniformly from U may not be easy, so we might instead define a Markov chain that will converge to this uniform distribution. Gibbs sampling is one possibility: We sample alternately from the conditional distribution for y given the current x — which is uniform over the interval $(0, f(x))$ — and from the conditional distribution for x given the current y — which is uniform over the region $S = \{\, x \;:\; y < f(x) \,\}$, which I call the 'slice' defined by y. Generating an independent point drawn uniformly from S may still be difficult, in which case we can substitute some update for x that leaves the uniform distribution over S invariant.

Similar auxiliary variable methods been used in the past. Higdon (1996) has interpreted the standard Metropolis algorithm in these terms. The highly successful Markov chain algorithm for the Ising model due to Swendsen and Wang (1987) can also be seen as an auxiliary variable method, which has been generalized by Edwards and Sokal (1988). In their scheme, the density (or probability mass) function is proportional to a product of k functions: $p(x) \propto f_1(x) \cdots f_k(x)$. They introduce k auxiliary variables, $y_1, \ldots, y_k$, and define a joint distribution for $(x, y_1, \ldots, y_k)$ which is uniform over the region where $0 < y_i < f_i(x)$ for $i = 1, \ldots, k$. Gibbs sampling, or some related Markov chain procedure, can then be used to sample for $(x, y_1, \ldots, y_k)$, much as described above for the case of a single auxiliary variable. Applications of such methods to image analysis have been discussed by Besag and Green (1993) and by Higdon (1996).

Mira and Tierney (in press) have shown that these auxiliary variable methods, with one or with many auxiliary variables, are uniformly ergodic under certain conditions. Roberts and Rosenthal (1999) have shown that these methods are geometrically ergodic under weaker conditions, and have also found some quantitative convergence bounds. These results all assume that the sampler generates a new value for x that is uniformly drawn from S, independently of the old value, which is often difficult in practice.

Concurrently with the work reported here[1], Damien, Wakefield, and Walker (in press) have viewed methods based on multiple auxiliary variables as a general approach to constructing Markov chain samplers for Bayesian inference problems. They illustrate how one can often decompose $f(x)$ into a product of k factors for which the intersection of the sets $\{\, x \,:\, y_i < f_i(x) \,\}$ is easy to compute. This leads to an easily implemented sampler, but convergence is slowed by the presence of many auxiliary variables. For example, for a model of k i.i.d. data points, one simple approach (similar to some examples of Damien, *et al*) is to have a factor (and auxiliary variable) for each data point, with the product of these factors being the likelihood. (Suppose for simplicity that the prior is uniform, and so needn't be represented in the posterior density.) For many models, finding $\{\, x \,:\, y_i < f_i(x) \,\}$ will be easy to compute when f_i is the likelihood from one data point. However, if this approach is applied to n data points that are modeled as coming from a Gaussian distribution with mean μ and variance 1, it is easy to see that after the y_i are chosen, the allowable range for μ will have width of order $1/n$. Since the width of the posterior distribution for μ will be of order $1/\sqrt{n}$, and since the posterior will be explored by a random walk, the convergence time will be of order n. Gibbs sampling would, of course, converge in a single iteration when there is only one parameter, and the slice sampling methods of this paper would also converge very rapidly for this problem, for any n. Using a large number of auxiliary variables is a costly way to avoid difficult computations.

I therefore am concerned in this paper with methods based on slice sampling with a single auxiliary variable. So that these methods will be practical for a wide range of problems, they often use updates for x that do not produce a point drawn independently from the slice, S, but merely change x in some fashion that leaves the uniform distribution over S invariant. This allows the methods to be used for any continuous distribution, provided only that we can compute some function, $f(x)$, that is proportional to the density.

4 Single-variable slice sampling methods

Slice sampling is simplest when only one (real-valued) variable is being updated. This will of course be the case when the distribution of interest is univariate, but more typically, the single-variable slice sampling methods of this section will be used to sample from a multivariate distribution for $x = (x_1, \ldots, x_n)$ by sampling repeatedly for each variable in turn. To update x_i, we must be able to compute a function, $f_i(x_i)$, that is proportional to $p(x_i \,|\, \{x_j\}_{j \neq i})$, where $\{x_j\}_{j \neq i}$ are the values of the other variables. Often, the joint distribution for $x_1, \ldots, x_n$ will be defined by some function, $f(x_1, \ldots, x_n)$, that is proportional to the joint density, in which case we can simply take $f_i(x_i) = f(\ldots, x_i, \ldots)$, where the variables other than x_i are fixed to their current values.

To simplify notation, I will here write the single real variable being updated as x (with subscripts denoting different such points, not components of x). I will write $f(x)$ for the

[1] An earlier version of this paper, under the title "Markov chain Monte Carlo methods based on 'slicing' the density function" was issued in November 1997 as Technical Report 9722, Department of Statistics, University of Toronto (available from my web page). It contains essentially all the material in this paper with the exception of Sections 5 and 8. The first application of the methods developed here, by Frey (1997), predates this technical report, referencing it as being 'in preparation'.

function proportional to the probability density of x. The single-variable slice sampling methods discussed here replace the current value, x_0, with a new value, x_1, found by a three-step procedure:

a) Draw a real value, y, uniformly from $(0, f(x_0))$, thereby defining a horizontal 'slice': $S = \{\, x : y < f(x) \,\}$. Note that x_0 is always within S.

b) Find an interval, $I = (L, R)$, around x_0 that contains at least a big part of the slice.

c) Draw the new point, x_1, from the part of the slice within this interval (ie, from $S \cap I$).

Step *(a)* picks a value for the auxiliary variable that is characteristic of slice sampling. Note that there is no need to retain this auxiliary variable from one iteration of the Markov chain to the next, since its old value is forgotten at this point anyway. In practice, it is often safer to compute $g(x) = \log(f(x))$ rather than $f(x)$ itself, in order to avoid possible problems with floating-point underflow. One can then use the auxiliary variable $z = \log(y) = g(x_0) - e$, where e is exponentially distributed with mean one, and define the slice by $S = \{\, x : z < g(x) \,\}$.

Steps *(b)* and *(c)* can potentially be implemented in several ways, which must of course be such that the resulting Markov chain leaves the distribution defined by $f(x)$ invariant. Figure 1 illustrates one generally-applicable method, in which the interval is found by 'stepping out', and the new point is drawn with a 'shrinkage' procedure. Figure 2 illustrates an alternative 'doubling' procedure for finding the interval. These and some other variations are described in detail next, followed by a proof that the resulting transitions leave the correct distribution invariant. I then describe some shortcuts that are possible when the distribution is unimodal.

4.1 Finding an appropriate interval

After a value for the auxiliary variable has been drawn, defining the slice S, the next task is to find an interval $I = (L, R)$, containing the current point, x_0, from which the new point, x_1, will be drawn. We would like this interval to contain as much of the slice as is feasible, so as to allow the new point to differ as much as possible from the old point, but we would also like to avoid intervals that are much larger than the slice, as this will make the subsequent sampling step less efficient.

Several schemes for finding an interval are possible:

1) Ideally, we would set $L = \inf(S)$ and $R = \sup(S)$. That is, we would set I to the smallest interval that contains the whole of S. This may not be feasible, however.

2) If the range of x is bounded, we might simply let I be that range. However, this may not be good if the slice is typically much smaller than the range.

3) Given an estimate, w, for the scale of S, we can randomly pick an initial interval of size w, containing x_0, and then perhaps expand it by a 'stepping out' procedure.

4) Similarly, we can randomly pick an initial interval of size w, and then expand it by a 'doubling' procedure.

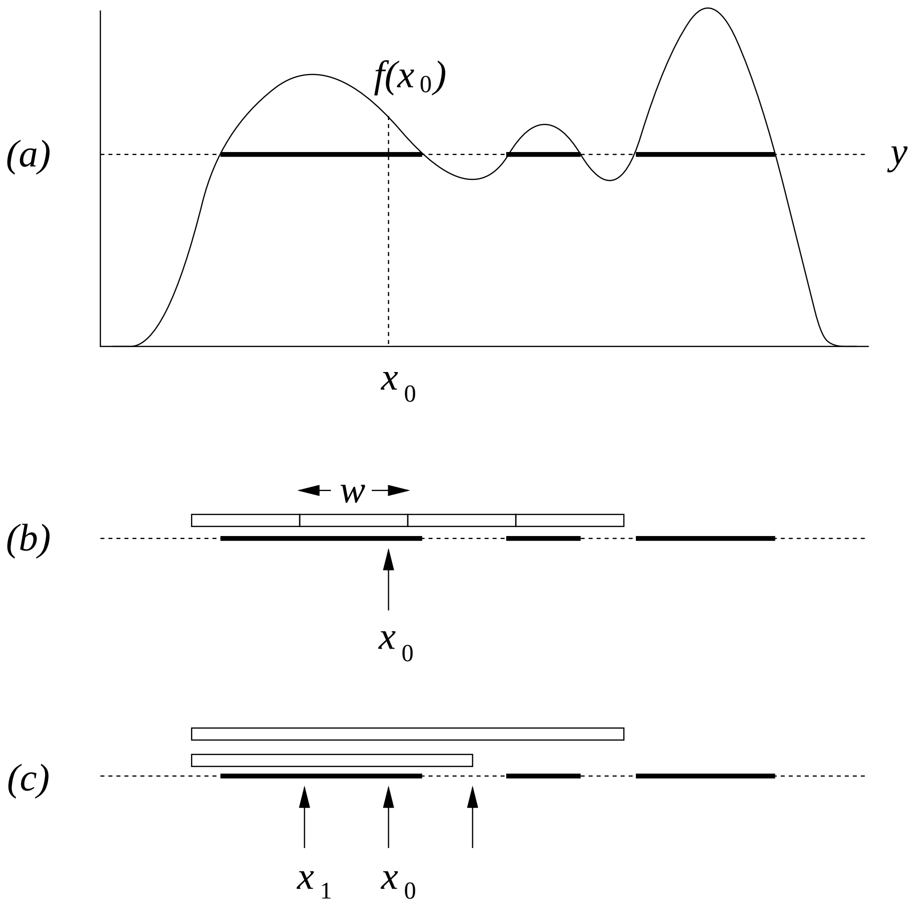

Figure 1: A single-variable slice sampling update using the stepping-out and shrinkage procedures. A new point, x_1, is selected to follow the current point, x_0, in three steps. *(a)* A vertical level, y, is drawn uniformly from $(0, f(x_0))$, and used to define a horizontal 'slice', indicated in bold. *(b)* An interval of width w is randomly positioned around x_0, and then expanded in steps of size w until both ends are outside the slice. *(c)* A new point, x_1, is found by picking uniformly from the interval until a point inside the slice is found. Points picked that are outside the slice are used to shrink the interval.

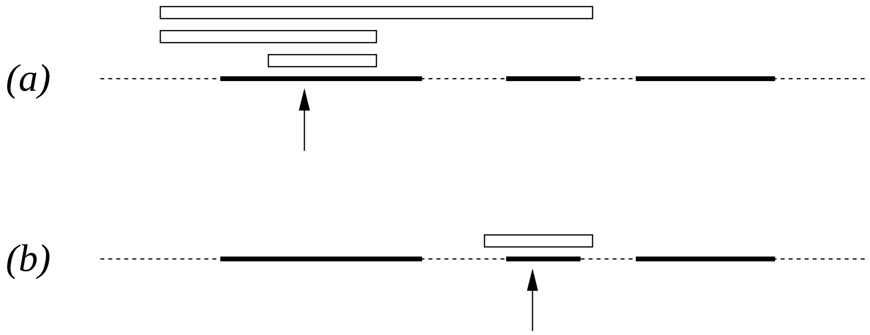

Figure 2: The doubling procedure. In *(a)*, the initial interval is doubled twice, until both ends are outside the slice. In *(b)*, where the start state is different, no doubling is done.

For each scheme, we must also be able to find the set A of acceptable successor states, defined as follows:

$$A \;=\; \{\, x \,:\, x \in S \cap I \text{ and } P(\text{Select } I \mid \text{At state } x) = P(\text{Select } I \mid \text{At state } x_0)\,\} \quad (3)$$

That is, A is the set of states from which we would be as likely to choose the interval I as we were to choose this I from the current state. When we subsequently sample from within I (see section 4.2), we will ensure that the state chosen is in A, a fact which will be used in the proof of correctness in section 4.3. Clearly, for schemes (1) and (2), $A = S$. For scheme (3), we will arrange that $A = S \cap I$. Things are not so simple for scheme (4), for which a special test of whether a state is in A may be necessary.

Scheme (1), in which I is set to the smallest interval containing S, will be feasible when all solutions of $f(x) = y$ can be found analytically, or by an efficient and robust numerical method, but one cannot expect this in general. Often, even the number of disjoint intervals making up S will be hard to determine.

Scheme (2) is certainly easy to implement when the range of x is bounded, and one can of course always arrange this by applying a suitable transformation. However, if the slice is usually much smaller than the full range, the subsequent sampling (see section 4.2) will be inefficient. This scheme has been used by Frey (1997).

The 'stepping out' procedure (scheme (3) above) is appropriate for any distribution, provided that some rough estimate, w, for the typical width of the slice is available. The manner in which an interval is found by stepping out is illustrated in Figure 1(b) and the procedure is given in detail in Figure 3. The size of the interval found can be limited to mw, for some specified integer m, or the interval can be allowed to grow to any size (ie, m can be set to infinity), in which case the procedure can be simplified in an obvious way (eliminating all references to J and K). Note that the random positioning of the initial interval and the random apportioning of the maximum number of steps m into a limit on going to the left and a limit on going to the right are essential for correctness, as they ensure that the final interval could equally well have been produced from any point within $S \cap I$.

If m is set to one in the stepping out procedure, the interval will always be of size w, and there will be no need to evaluate f at its endpoints. This saves some computation time, but is undesirable if w might be much too small.

The 'doubling' procedure (scheme (4) above) can expand the interval faster than the stepping out procedure, and hence may be more efficient when the estimated size of the slice (w) turns out to be too small. This procedure is illustrated in Figure 2, and given in detail in Figure 4. Doubling produces a sequence of intervals, each twice the size of the previous one, until an interval is found with both ends outside the slice, or a predetermined limit is reached. Note that when the interval is doubled the two sides are not expanded equally. Instead just one side is expanded, chosen at random (irrespective of whether that side is already outside the slice). This is essential to the correctness of the method, since it produces a final interval that could have been obtained from points other than the current one. The set A of acceptable next states is restricted to those for which the same interval could have been produced, and is in general not all of $S \cap I$. This complicates the subsequent sampling somewhat, as described below.

```
Input:    $f$   = function proportional to the density
          $x_0$ = the current point
          $y$   = the vertical level defining the slice
          $w$   = estimate of the typical size of a slice
          $m$   = integer limiting the size of a slice to $mw$

Output:   $(L, R)$ = the interval found

$U \sim \text{Uniform}\,(0,1)$
$L \leftarrow x_0 - w * U$
$R \leftarrow L + w$

$V \sim \text{Uniform}\,(0,1)$
$J \leftarrow \text{Floor}\,(m * V)$
$K \leftarrow (m-1) - J$

repeat while $J > 0$ and $y < f(L)$:
    $L \leftarrow L - w$
    $J \leftarrow J - 1$

repeat while $K > 0$ and $y < f(R)$:
    $R \leftarrow R + w$
    $K \leftarrow K - 1$
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Figure 3: The 'stepping out' procedure for finding an interval around the current point. The notation $U \sim \text{Uniform}\,(0,1)$ indicates that U is set to a number randomly drawn from the uniform distribution on $(0,1)$.

```
Input:    $f$   = function proportional to the density
          $x_0$ = the current point
          $y$   = the vertical level defining the slice
          $w$   = estimate of the typical size of a slice
          $p$   = integer limiting the size of a slice to $2^p w$

Output:   $(L, R)$ = the interval found

$U \sim \text{Uniform}\,(0,1)$
$L \leftarrow x_0 - w * U$
$R \leftarrow L + w$
$K \leftarrow p$

repeat while $K > 0$ and $\{\ y < f(L)$ or $y < f(R)\ \}$:
    $V \sim \text{Uniform}\,(0,1)$
    if $V < 1/2$ then $L \leftarrow L - (R-L)$
                 else $R \leftarrow R + (R-L)$
    $K \leftarrow K - 1$
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Figure 4: The 'doubling' procedure for finding an interval around the current point. Note that it is possible to save some computation in second and later iterations of the loop, since only one of $f(L)$ and $f(R)$ will have changed from the previous iteration.

4.2 Sampling from the part of the slice within the interval

Once an interval, $I = (L, R)$, has been found containing the current point, x_0, the final step of the single-variable slice sampling procedure is to randomly draw a new point, x_1, from within this interval. This point must lie within the set A of points acceptable as the next state of the Markov chain, defined in equation (3).

Two methods could be used to sample from I:

i) Repeatedly sample uniformly from I until a point is drawn that lies within A.

ii) Repeatedly sample uniformly from an interval that is initially equal to I, and which shrinks each time a point is drawn that is not in A, until a point within A is found.

Method *(i)* could potentially be very inefficient, if ever A turns out to be a tiny portion of I. The shrinkage of the interval in method *(ii)* ensures that the expected number of points drawn will not be too large, making this a more appropriate method for general use.

The shrinkage procedure is shown in detail in Figure 5. Note that each rejected point is used to shrink the interval in such a way that the current point remains within it. Since the current point is always within A, the interval used always contains acceptable points, ensuring that the procedure will terminate.

If the interval was found by scheme (1), (2), or (3), the set A is simply $S \cap I$. However, if the doubling procedure (scheme (4)) was used, A may be a smaller subset of $S \cap I$. This is illustrated in Figure 2. In 2(a), an interval is found by doubling an initial interval until both ends are outside the slice. A different starting point is considered in 2(b), one which might have been drawn from the interval found in 2(a). The doubling procedure terminates earlier starting from here, so this point is not in A. (Note that A is here defined conditional on the alignment of the initial interval.)

The Accept (x_1) predicate in Figure 6 tests whether a point in $S \cap I$ is in A when the doubling procedure (scheme (4)) was used. This procedure works backward through the intervals that the doubling procedure would pass through to arrive at I when starting from the new point, checking that none of them have both ends outside the slice, which would lead to earlier termination of the doubling procedure. (Note that one needn't check this explicitly until the intervals differ from those followed from the current point, a condition tracked with the variable D in the procedure.) If the distribution is known to be unimodal, this test can be omitted, as discussed in section 4.4.

4.3 Correctness of single-variable slice sampling

To show that single-variable slice sampling is a correct procedure, we must show that each update leaves the desired distribution invariant. To guarantee convergence to this distribution, the resulting Markov chain must also ergodic. This is not always true, but it is in those situations (such as when $f(x) > 0$ for all x) for which one can easily show that Gibbs sampling is ergodic. I will not discuss the more difficult situations here.

To show invariance, we suppose that the initial state, x_0, is distributed according to $f(x)$. In step *(a)* of single-variable slice sampling, a value for y is drawn uniformly from $(0, f(x))$.

```
Input:   $f$      =  function proportional to the density
         $x_0$    =  the current point
         $y$      =  the vertical level defining the slice
         $w$      =  estimate of the typical size of a slice
         $(L, R)$ =  the interval to sample from

Output:  $x_1$    =  the new point

$\bar{L} \leftarrow L, \quad \bar{R} \leftarrow R$

repeat:
    $U \sim \text{Uniform}\,(0,1)$
    $x_1 \leftarrow \bar{L} + U * (\bar{R} - \bar{L})$
    if $y < f(x_1)$ and Accept $(x_1)$ then exit loop
    if $x_1 < x_0$ then $\bar{L} \leftarrow x_1$ else $\bar{R} \leftarrow x_1$
```

Figure 5: The 'shrinkage' procedure for sampling from the interval. The notation Accept (x_1) represents a test for whether a point, x_1, that is within $S \cap I$ is an acceptable next state. If scheme (1), (2), or (3) was used for constructing the interval, all points within $S \cap I$ are acceptable. If the doubling procedure (scheme (4)) was used, the point must pass the test of Figure 6, below.

```
Input:   $f$      =  function proportional to the density
         $x_0$    =  the current point
         $x_1$    =  the possible next point
         $y$      =  the vertical level defining the slice
         $w$      =  estimate of the typical size of a slice
         $(L, R)$ =  the interval found by the doubling procedure

Output:  whether or not $x_1$ is an acceptable next state

$\hat{L} \leftarrow L, \quad \hat{R} \leftarrow R$
$D \leftarrow$ false

repeat while $\hat{R} - \hat{L} > 1.1 * w$:
    $M \leftarrow (\hat{L} + \hat{R}) / 2$
    if $\{ x_0 < M$ and $x_1 \geq M \}$ or $\{ x_0 \geq M$ and $x_1 < M \}$ then $D \leftarrow$ true
    if $x_1 < M$ then $\hat{R} \leftarrow M$ else $\hat{L} \leftarrow M$
    if $D$ and $y \geq f(\hat{L})$ and $y \geq f(\hat{R})$ then
        The new point is not acceptable

The new point is acceptable if not rejected in the loop above
```

Figure 6: The test for whether a new point, x_1, that is within $S \cap I$ is an acceptable next state, when the interval was found by the 'doubling' procedure. The multiplication by 1.1 in the 'while' condition guards against possible round-off error.

The joint distribution for x_0 and y will therefore be as in equation (1). If the subsequent steps update x_0 to x_1 in a manner that leaves this joint distribution invariant, then when we subsequently discard y, the resulting distribution for x_1 will be the marginal of this joint distribution, which is the same as that defined by $f(x)$, as desired.

We therefore need only show that the selection of x_1 to follow x_0 in steps *(b)* and *(c)* of the single-variable slice sampling procedure leaves the joint distribution of x and y invariant. Since these steps do not change y, this is the same as leaving the conditional distribution for x given y invariant, and this conditional distribution is uniform over $S = \{\, x : y < f(x) \,\}$, the slice defined by y. We can show invariance of this distribution by showing that the updates satisfy detailed balance, which for a uniform distribution reduces to showing that the probability density for x_1 to be selected as the next state, given that the current state is x_0, is the same as the probability density for x_0 to be the next state, given that x_1 is the current state, for any states x_0 and x_1 within S.

In the process of picking a new state, various intermediate choices are made randomly. When the interval is found by the stepping out procedure of Figure 3, the alignment of the initial interval is randomly chosen, as is the division of the maximum number of intervals into those used to extend to the left and those used to extend to the right. For the doubling procedure of Figure 4, the alignment of the initial interval is random and the decisions whether to extend to the right or to the left are also made randomly. When sampling is done using the shrinkage procedure of Figure 5, zero or more rejected points will be chosen before the final point. Let r denote these intermediate random choices. I will prove that detailed balance holds for the entire procedure by showing the following stronger result:

$$\begin{aligned} & P(\text{next state} = x_1,\ \text{intermediate choices} = r \mid \text{current state} = x_0) \\ = \ & P(\text{next state} = x_0,\ \text{intermediate choices} = \pi(r) \mid \text{current state} = x_1) \end{aligned} \tag{4}$$

where $\pi(r)$ is some one-to-one mapping that has Jacobian one (with regard to the real-valued variables), which may depend on x_0 and x_1. Integrating over all possible values for r then gives the desired result.

In detail, the mapping π used is as follows. First, if the interval I is found by the stepping out or doubling procedure, an intermediate value, U, will be generated by the procedure of Figure 3 or 4, and used to define the initial interval. We define π so that it maps the value U_0 chosen when the state is x_0 to the following U_1 when the state is x_1:

$$U_1 \ = \ \text{Frac}\,(U_0 + (x_1 - x_0)/w) \tag{5}$$

where $\text{Frac}\,(x) = x - \text{Floor}\,(x)$ is the fractional part of x. This mapping associates values that produce the same alignment of the initial interval. Note also that it has Jacobian one. If the stepping out procedure is used, a value for J is also generated, uniformly from the set $\{\, 0, \ldots, m{-}1 \,\}$. The mapping π associates the J_0 found when the state is x_0 with the following J_1 when the state is x_1:

$$J_1 \ = \ J_0 \ + \ (x_1/w - U_1) \ - \ (x_0/w - U_0) \tag{6}$$

Here, $(x_1/w - U_1) \ - \ (x_0/w - U_0)$ is an integer giving the number of steps (of size w) from the left end of the interval containing x_0 to the left end of the interval containing x_1. This is the amount by which we must adjust J_0 in order to ensures that if the interval found starting from x_0 grows to its maximum size, the associated interval found starting from x_1 will be identical. Similarly, if the doubling procedure of Figure 4 is used, the sequence of random decisions as to which side of the interval to expand is mapped by π to the sequence of decisions that would cause the interval expanding from x_1 to become identical to the interval expanding from x_0 when the latter first includes x_1, and to remain identical through further expansions. Note in this respect that there is at most one way that an given final interval can be obtained by successive doublings from a given initial interval, and that the alignment of the initial intervals by the association of U_0 with U_1 ensures that doubling starting from x_1 can indeed lead to the same interval as found from x_0. Finally, to complete the definition, π maps the sequence of rejected points used to shrink the interval found from x_0 (see Figure 5) to the same sequence of points when x_1 is the start state.

It remains to show that with this definition of π, equation (4) does indeed hold, for all points x_0 and x_1, and all possible intermediate values r. The equation certainly holds when both sides are zero, so we needn't consider situations where movement between x_0 and x_1 is impossible (in conjunction with the given intermediate values).

Consider first the probability (density) for producing the intermediate values that define the interval I. For the stepping out and doubling procedures, the values U_0 and U_1 (related by π) that are generated from x_0 and x_1 will certainly have the same probability density, since U is drawn from a uniform distribution. Similarly, for the stepping out procedure, the values J_0 and J_1 are drawn from a uniform distribution over $\{0, \ldots, m-1\}$, and hence have the same probability as long as J_0 and J_1 are both in this set, which will be true whenever movement between x_0 and x_1 is possible. For the doubling procedure, a sequence of decisions as to which side to extend is made, with all sequences of a given length having the same probability. Here also, the sequences associated by π will have the same probability, *provided* the same number of doublings are done starting from x_0 as from x_1. This need not be true in general, but if the sequence from x_1 is shorter, the test of Figure 6 will eliminate x_1 as a possible successor to x_0, and if the sequence from x_0 is shorter, x_1 will not be a possible successor because it will be outside the interval I found from x_0. Both sides of equation 4 will therefore be zero in this situation.

Note next that the intervals found by any of the schemes of section 4.1 will be the same for x_0 as for x_1, when the intermediate values chosen are related by π, assuming a transition from x_0 to x_1 is possible. For the stepping out procedure, the maximum extent of the intervals will be the same because of the relationships between U_0 and U_1 and between J_0 and J_1. Furthermore, the actual intervals found by stepping out (limited by the maximum) must also be the same whenever a transition between x_0 and x_1 is possible, since if the interval starting from x_0 has reached x_1, expansion of both intervals will continue in the same direction until the outside of the slice or the maximum is reached, and likewise in the other direction. Similarly, the mapping π is defined to be such that if the interval found by the doubling procedure starting from x_0 includes x_1, the same interval would be found from x_1, provided the process was not terminated earlier (by both ends being outside the slice), in which case x_1 is not a possible successor (as it would be rejected by the procedure of Figure 6). Note also that since the set A is determined by I (for any start state), it too will be the same for x_0 as for x_1.

If we sample from this I by simple rejection (scheme *(i)* in section 4.2), the state chosen will be uniformly distributed over A, so the probability of picking x_0 will be the same as that of picking x_1. If we instead use the shrinkage procedure (scheme *(ii)*, in Figure 5), we need to consider as intermediate values the sequence of rejected points that were used to narrow the interval (recall that under π this sequence is the same for x_0 as for x_1). The probability density for the first of these is clearly the same for both starting points, since I is the same. As the interval shrinks, it remains the same for both x_0 and x_1, since the rejection decisions (based on A) are the same, and since we need consider only the case where the same end of the interval is moved to the rejected point (as otherwise a transition between x_0 and x_1 in conjunction with these intermediate values would be impossible). The probability densities for later rejected points, and for the final accepted state, are therefore also the same.

This completes the proof. Various seemingly reasonable modifications — such as changing the doubling procedure of Figure 4 to not expand the interval on a side that is already outside the slice — would undermine the argument of the proof, and hence cannot be used. However, some shortcuts are allowed when the distribution is unimodal, as discussed next.

4.4 Shortcuts for unimodal distributions

Certain shortcuts can be used when the conditional distribution for the variable being updated is known to be unimodal, or more generally, when the slice, S, is known to consist of a single interval. For some values of the auxiliary variable, S may be a single interval even when the distribution is multimodal, but the effort required to confirm this probably exceeds the gain from using the shortcuts, so I will refer only to the unimodal case here.

Two shortcuts apply when the 'doubling' procedure is used to find the interval. First, for a unimodal distribution, the acceptance test in Figure 6 can be omitted, since it will always indicate that the new point is acceptable. To see this, note that the procedure rejects a point when one of the intervals found by doubling from that starting point has both ends outside the slice, but does not contain the current point. Since both the current point and the new point are inside the slice, this is impossible if the slice consists of only one interval.

Second, the interval found by the doubling procedure can sometimes be shrunk at the outset. The side chosen for extension when the interval doubles will sometimes be outside the slice already. When the distribution is known to be unimodal, it is not possible for such an extension to contain any points within the slice. Accordingly, before sampling is begun, the endpoints of the interval can be set to the first point in each direction that was found to lie outside the slice. This may reduce the number of points generated, while having no effect on the distribution of the point finally chosen.

Finally, if the distribution is known to be unimodal *and* no limit is imposed on the size of the interval found (ie, m and p in Figures 3 and 4 are infinite), the estimate, w, for the typical size of a slice can be set on the basis of past iterations. One could, for example, keep a running average of the distance between the old and new points in past iterations, and use this (or some suitable multiple) as the estimate w. This is valid because the distribution of the new point does not depend on w in this situation, even though w influences how efficiently this new point is found. Indeed, when the distribution is known to be unimodal, one can use any method at all for finding an interval that contains the current point and has both ends outside the slice, as any such interval will lead to the new point finally chosen being drawn uniformly from the slice.

5 Multivariate slice sampling methods

Rather than sample from a distribution for $x = (x_1, \ldots, x_n)$ by applying one of the single-variable slice sampling procedures described above to each x_i in turn, we might try instead to apply the idea of slice sampling directly to the multivariate distribution. I will start by describing a straightforward generalization of the single-variable methods to multivariate distributions, and then describe a more sophisticated method, which can potentially allow for adaptation to the local dependencies between variables.

5.1 Multivariate slice sampling with hyperrectangles

We can generalize the single-variable slice sampling methods of Section 4 to methods for performing multivariate updates by replacing the interval $I = (L, R)$ by an axis-aligned hyperrectangle $H = \{x : L_i < x_i < R_i \text{ for all } i = 1, \ldots, n\}$. Here, L_i and R_i define the extent of the hyperrectangle along the axis for variable x_i.

The procedure for finding the next state, $x_1 = (x_{1,1}, \ldots, x_{1,n})$, from the current state, $x_0 = (x_{0,1}, \ldots, x_{0,n})$, parallels the single-variable procedure:

a) Draw a real value, y, uniformly from $(0, f(x_0))$, to define the slice $S = \{\, x : y < f(x) \,\}$.

b) Find a hyperrectangle, $H = (L_1, R_1) \times \cdots \times (L_n, R_n)$, around x_0, which preferably contains at least a big part of the slice.

c) Draw the new point, x_1, from the part of the slice within this hyperrectangle (ie, from $S \cap H$).

It would perhaps be ideal for step (b) to set H to the smallest hyperrectangle containing S, but this is unlikely to be feasible. An easy option when all the variables have bounded range is to set H to be the entire space, but this will often be rather inefficient, since S is likely to be much smaller.

In practice, we must usually be content to find an H that contains the current point, x_0, but probably not all of S, using width parameters, w_i, for the dimensions of H along each axis. If we know nothing about the relative scales of different variables, we might set all the w_i to a single scale parameter, w. The simplest way of finding H is to randomly position a hyperrectangle with these dimensions, uniformly over positions that lead to H containing x_0. This generalizes the random positioning of the initial interval I for the single-variable slice sampling methods. The stepping out and doubling procedures used with single-variable slice sampling do not generalize so easily, however. The goal of finding an interval whose endpoints are outside the slice would generalize to finding a hyperrectangle all of whose vertices are outside the slice, but since an n dimensional hyperrectangle has 2^n vertices,

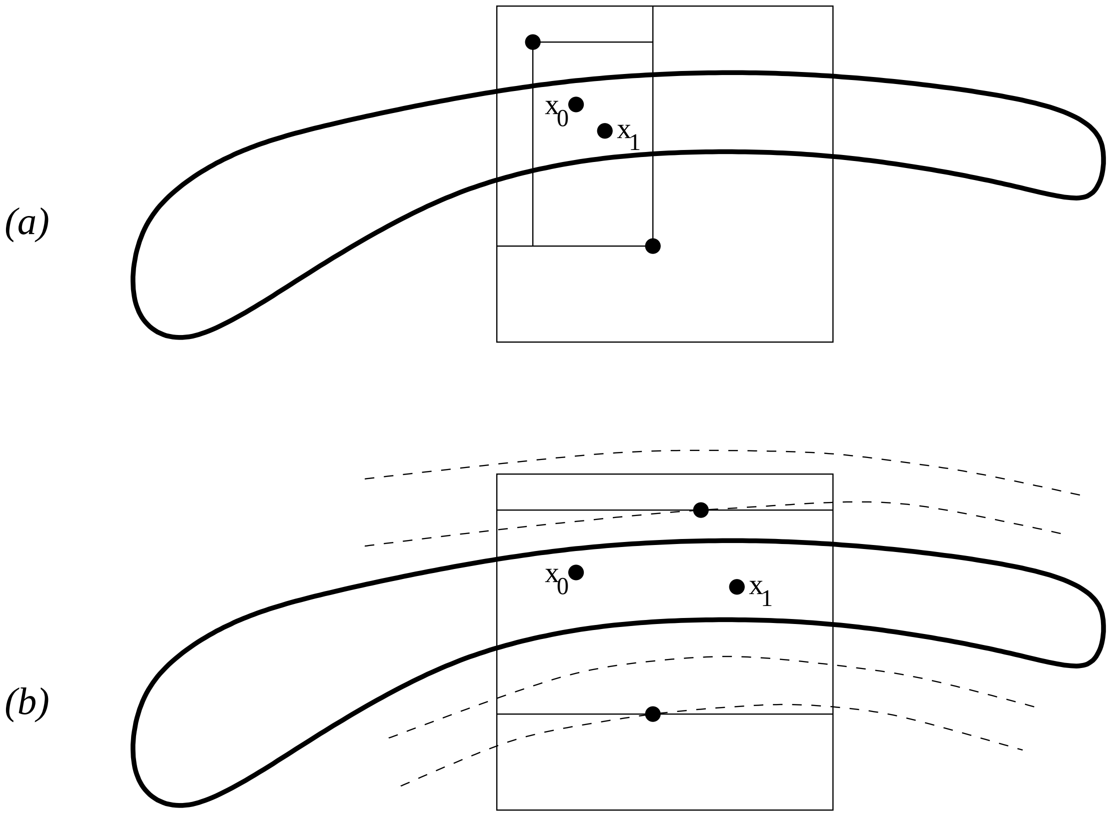


Figure 7: Multivariate slice sampling with hyperrectangles. The heavy line outlines the slice, containing the current point, x_0. The large square is the initial hyperrectangle. In (a), the hyperrectangle is shrunk in all directions when the point drawn is outside the slice, until a new point, x_1, inside the slice is found. In (b), the hyperrectangle is shrunk along only one axis, determined from the gradient and the current dimensions of the hyperrectangle. The dashed lines are contours of the density function, indicating the direction of the gradient.

we would certainly not want to test for this when n is large. The stepping out procedure seems to be too time consuming in any case, since one would need to step out in each of the n directions. The doubling procedure does generalize appropriately, and one could decide to stop doubling when a randomly-drawn point picked uniformly from the current hyperrectangle is outside the slice. This idea is worth exploring, but here I will consider only the simplest scheme, which is to use the randomly positioned hyperrectangle without any expansion, though it is then crucial that the w_i not be much smaller than they should be.

The shrinkage procedure of Figure 5 generalizes easily to multiple dimensions — the hyperrectangle can simply be shrunk independently along each axis. Combining this with simple random positioning of H, one gets the multivariate slice sampling method shown in Figure 7(a), and given in detail in Figure 8. The validity of this method can be proven in the same way as was done for single-variable slice sampling in Section 4.3.

Although this simple multivariate slice sampling method is easily implemented, and will often be reasonably efficient, in one respect it works less well than applying single-variable slice sampling to each variable in turn. When each variable is updated separately, the

```
Input:   $f$ = function proportional to the density
         $x_0$ = the current point, of dimension $n$
         $w_i$ = scale estimates for each variable, $i = 1, \ldots, n$

Output:  $x_1$ = the new point

Step (a): Find the value of y that defines the slice.

$y \sim \text{Uniform}\,(0,\ f(x_0))$

Step (b): Randomly position the hyperrectangle $H = (L_1, R_1) \times \cdots \times (L_n, R_n)$.

For $i = 1$ to $n$:
    $U_i \sim \text{Uniform}\,(0, 1)$
    $L_i \leftarrow x_{0,i} - w_i * U_i$
    $R_i \leftarrow L_i + w_i$

Step (c): Sample from H, shrinking when points are rejected.

Repeat:
    For $i = 1$ to $n$:
        $U_i \sim \text{Uniform}\,(0, 1)$
        $x_{1,i} \leftarrow L_i + U_i * (R_i - L_i)$

    if $y < f(x_1)$ then exit loop

    For $i = 1$ to $n$:
        if $x_{1,i} < x_{0,i}$ then $L_i \leftarrow x_{1,i}$ else $R_i \leftarrow x_{1,i}$
```

Figure 8: A simple multivariate slice sampling procedure, with randomly positioned hyperrectangle, and shrinkage in all directions.

interval for that variable will be shrunk only as far as needed in order to obtain a new value within the slice. The amount of shrinkage can be different for different variables. In contrast, the procedure of Figure 8 shrinks all dimensions of the hyperrectangle until a point inside the slice is found, even though the probability density may not vary rapidly in some of these dimensions, making shrinkage in these directions unnecessary (and undesirable).

One way to try to avoid this problem is illustrated in Figure 7(b). Rather than shrink all dimensions of the hyperrectangle when the last point chosen was outside the slice, we can instead shrink along only one axis, basing the choice on the gradient of $\log f(x)$, evaluated at the last point. Specifically, only the axis corresponding to variable x_i is shrink, where i maximizes the following product:

$$(R_i \,-\, L_i)\; |G_i| \tag{7}$$

where G is the gradient of $\log f(x)$ at the last point chosen. By multiplying the magnitude of component i of the gradient by the width of the hyperrectangle in this direction, we get an estimate of the amount by which $\log f(x)$ changes along axis i. The axis for which this change is thought to be largest is likely to be the best one to shrink in order to eliminate points outside the slice. Unfortunately, if this decision were based as well on whether the sign of the gradient indicates that $\log f(x)$ is increasing or decreasing as we move toward the current point, x_0, the shrinkage decision might be different if we were to shrink from the final accepted point, x_1, which would invalidate the method (unless we somehow avoided or rejected such points).

Many more elaborate schemes along these lines are possible. For instance, we might shrink along all axes for which the product (7) is greater than some threshold. A good scheme might preserve the ability of single-variable slice sampling to adapt differently for different variables, while keeping the advantages that simultaneous updates may sometimes have (eg, in producing an ergodic chain when there are tight dependencies between variables).

More ambitiously, we might hope that a multivariate slice sampler could adapt to the dependencies between variables, not just to their different scales. This will require that we go beyond axis-aligned hyperrectangles, as is done in the next section.

5.2 A framework for adaptive multivariate slice sampling

We would like a more general framework by which trial points outside the slice that were previously rejected can be used to guide the selection of future trial points. In contrast to schemes based on hyperrectangles, we would like future trial points to potentially come from distributions that take account of the dependencies between variables. The scheme I present here achieves this by laying down a trail of ‘crumbs’ that guide the selection of future trial points, leading eventually to a point inside the slice. A crumb can be anything — eg, a discrete value, a real number, a vector, a hyperrectangle — but the method is perhaps most easily visualized when crumbs are points in the state space being sampled from.

As with the previous slice sampling schemes, we start by chosing a value y uniformly between zero and $f(x_0)$, where x_0 is the current point. A crumb, c_1, is then draw at random from some distribution with density (or probability mass) function $g_1(c;\, x_0,\, y)$.

Note that this distribution may depend on both the current point, x_0, and on the value of y that defines the slice. A first trial point, x_1^*, is then drawn from the distribution with density $h_1(x^*;\, y,\, c_1) = g_1(c_1;\, x^*,\, y) \,/\, Z_1(y,\, c_1)$, where $Z_1(y,\, c_1) = \int g_1(c_1;\, x^*,\, y)\, dx^*$ is the appropriate normalizing constant. One can view x_1^* as being drawn from a pseudo-posterior distribution, based on a uniform prior, and the "data" that the first crumb was c_1. If x_1^* is inside the slice, we set the new point, x_1, to x_1^*, and are finished. Otherwise, a second crumb, c_2, is drawn from some distribution $g_2(c;\, x_0,\, y,\, c_1,\, x_1^*)$, which may depend on the previous crumb and the previous trial point, as well as x_0 and y. The second trial point is then drawn from the pseudo-posterior distribution based on the "data" c_1 and c_2 — that is, x_2^* is drawn from

$$h_2(x^*;\, y,\, c_1,\, x_1^*,\, c_2) \;=\; g_1(c_1;\, x^*,\, y)\, g_2(c_2;\, x^*,\, y,\, c_1,\, x_1^*) \,/\, Z_2(y,\, c_1,\, x_1^*,\, c_2) \tag{8}$$

where $Z_2(y,\, c_1,\, x_1^*,\, c_2) = \int g_1(c_1;\, x^*,\, y)\, g_2(c_2;\, x^*,\, y,\, c_1,\, x_1^*)\, dx^*$. If x_2^* is inside the slice, it becomes the new state. Otherwise, we draw a third crumb, from a distribution that may depend on the current state, the value defining the slice, the previous crumbs, and the previous trial points, generate a third trial point using this and the previous crumbs, and so forth until a trial point lying within the slice is found.

To show that this procedure leaves the distribution with density $f(x)/Z$ invariant, it suffices to show that it separately satisfies detailed balance with respect to transitions that occur in conjunction with any given number of crumbs being drawn. In the case, for instance, of transitions involving two crumbs, we can show this by showing the stronger property that for any x_1^* that is not in the slice defined by y and any x_2^* that is in this slice, the following will hold:

$$P(x_0)\; P(y,\, c_1,\, x_1^*,\, c_2,\, x_2^* \mid x_0) \;=\; P(x_2^*)\; P(y,\, c_1,\, x_1^*,\, c_2,\, x_0 \mid x_2^*) \tag{9}$$

Here, $P(x_0)$ and $P(x_2^*)$ are the probability densities for the current point and the point that will become the new point (which are proportional to $f(x)$). The conditional probabilities above are the densities for the given sequence of values being chosen during the procedure, given that the current point is the one conditioned on. The left side of equation (9) can be written as follows:

$$\begin{aligned}
&P(x_0) \cdot P(y \mid x_0) \cdot P(c_1 \mid x_0,\, y) \cdot P(x_1^* \mid y,\, c_1) \cdot P(c_2 \mid x_0,\, y,\, c_1,\, x_1^*) \cdot P(x_2^* \mid y,\, c_1,\, x_1^*,\, c_2) \\
&\quad = \; [f(x_0)/Z] \,\cdot\, [1/f(x_0)] \,\cdot\, g_1(c_1;\, x_0,\, y) \,\cdot\, [g_1(c_1;\, x_1^*,\, y) \,/\, Z_1(y,\, c_1)] \\
&\qquad\qquad \cdot\, g_2(c_2;\, x_0,\, y,\, c_1,\, x_1^*) \,\cdot\, [g_1(c_1;\, x_2^*,\, y)\, g_2(c_2;\, x_2^*,\, y,\, c_1,\, x_1^*) \,/\, Z_2(y,\, c_1,\, x_1^*,\, c_2)]
\end{aligned}$$

The right side is

$$\begin{aligned}
&P(x_2^*) \cdot P(y \mid x_2^*) \cdot P(c_1 \mid x_2^*,\, y) \cdot P(x_1^* \mid y,\, c_1) \cdot P(c_2 \mid x_2^*,\, y,\, c_1,\, x_1^*) \cdot P(x_0 \mid y,\, c_1,\, x_1^*,\, c_2) \\
&\quad = \; [f(x_2^*)/Z] \,\cdot\, [1/f(x_2^*)] \,\cdot\, g_1(c_1;\, x_2^*,\, y) \,\cdot\, [g_1(c_1;\, x_1^*,\, y) \,/\, Z_1(y,\, c_1)] \\
&\qquad\qquad \cdot\, g_2(c_2;\, x_2^*,\, y,\, c_1,\, x_1^*) \,\cdot\, [g_1(c_1;\, x_0,\, y)\, g_2(c_2;\, x_0,\, y,\, c_1,\, x_1^*) \,/\, Z_2(y,\, c_1,\, x_1^*,\, c_2)]
\end{aligned}$$

These are readily seen to be equal, as is true in general for transitions involving any number of crumbs.

The hyperrectangle methods of Section 5.1 can be viewed in this framework. The randomly placed initial hyperrectangle is the first crumb. The first trial point is chosen from those points that could produce this initial hyperrectangle, which is simply the set of points within the hyperrectangle. The second and later crumbs are the shrunken hyperrectangles. Conditional on the current point, the previous crumb (ie, the previous hyperrectangle), and the previous trial point, these have degenerate distributions, concentrated on a single hyperrectangle. The possible corresponding trial points are the points within the shrunken hyperrectangle.

By using different sorts of crumbs, and different distributions for them, a huge variety of methods could be constructed within this framework. I will here only briefly discuss methods in which the crumbs are points in the state space, and have multivariate Gaussian distributions. The distributions of the trial points given the crumbs will then also be multivariate Gaussians.

In the simplest method of this sort, every g_i is Gaussian with mean x_0 and covariance matrix $\sigma^2 I$, for some fixed σ^2. The distribution, h_i, for x_i^* will then be Gaussian with mean $\bar{c}_i = (c_1 + \ldots + c_i)/i$ and covariance matrix $(\sigma^2/i)I$. As more and more trial points are generated, they will come from narrower and narrower distributions, which will be concentrated closer and closer to the current point (since $\bar{c}_i$ will approach x_0). This is analogous to shrinkage in the hyperrectangle method. In practice, it would probably be desirable to let σ_i^2 decrease with i (perhaps exponentially), so that the trial points would be forced closer to x_0 more quickly. Alternatively, one might look at $f(x_{i-1}^*)/y$ in order to estimate what value for σ_i would produce a distribution for the next trial point, x_i^*, that is likely to lie within the slice.

More generally, g_i could be a multivariate Gaussian with mean x_0 and some covariance matrix Σ_i, which may depend on the value of y, the previous crumbs, and the previous trial points. In particular, Σ_i could depend on the gradients of $f(x_j^*)$ for $j < i$, which provide information on what Gaussian distribution would be a good local approximation to $f(x)$. The distribution, h_i, for trial point x_i^* will then have covariance $\Sigma_i^* = [\Sigma_1^{-1} + \cdots + \Sigma_i^{-1}]^{-1}$ and mean $\bar{c}_i = \Sigma_i^* \, [\Sigma_1^{-1} c_1 + \cdots + \Sigma_i^{-1} c_i]$.

When x is of only moderate dimensionality, explicitly performing operations involving these covariance matrices would be tolerable, and a wide variety of ways for producing Σ_i would be feasible. For higher-dimensional problems, such operations would need to be avoided, as is done in an optimization context with the conjugate gradient and other related methods. Further research is therefore needed in order to fully exploit the potential of this promising framework for adaptation, and to compare it with methods based on the 'delayed rejection' (also called 'splitting rejection') framework of Tierney and Mira (Mira 1998, Chapter 5; Tierney and Mira 1999).

6 Overrelaxed slice sampling

When the updates used do not account for the dependencies between variables, many updates will be needed to move from one part of the distribution to another. Sampling efficiency can be improved in this context by suppressing the random walk behaviour characteristic of simple schemes such as Gibbs sampling. One way of achieving this is by using 'overrelaxed' updates. Like Gibbs sampling, overrelaxation methods update each variable in turn, but rather than drawing a new value for a variable from its conditional distribution independently of the current value, the new value is instead chosen to be on the opposite side of the mode from the current value. In Adler's (1981) scheme, applicable when the conditional distributions are Gaussian, the new value for variable i is

$$x_i' \;=\; \mu_i + \alpha\,(x_i - \mu_i) + \sigma_i\,(1-\alpha^2)^{1/2}\,n \tag{10}$$

where μ_i and σ_i are the conditional mean and standard deviation of variable i, n is a Gaussian random variate with mean zero and variance one, and α is a parameter slightly greater than -1. This method is analysed and discussed by Barone and Frigessi (1990) and by Green and Han (1992), though these discussions fail in some respects to properly elucidate the true benefits and limitations of overrelaxation (Neal 1998). The crucial ability of overrelaxation to (sometimes) suppress random walks is illustrated for a bivariate Gaussian distribution in Figure 9.

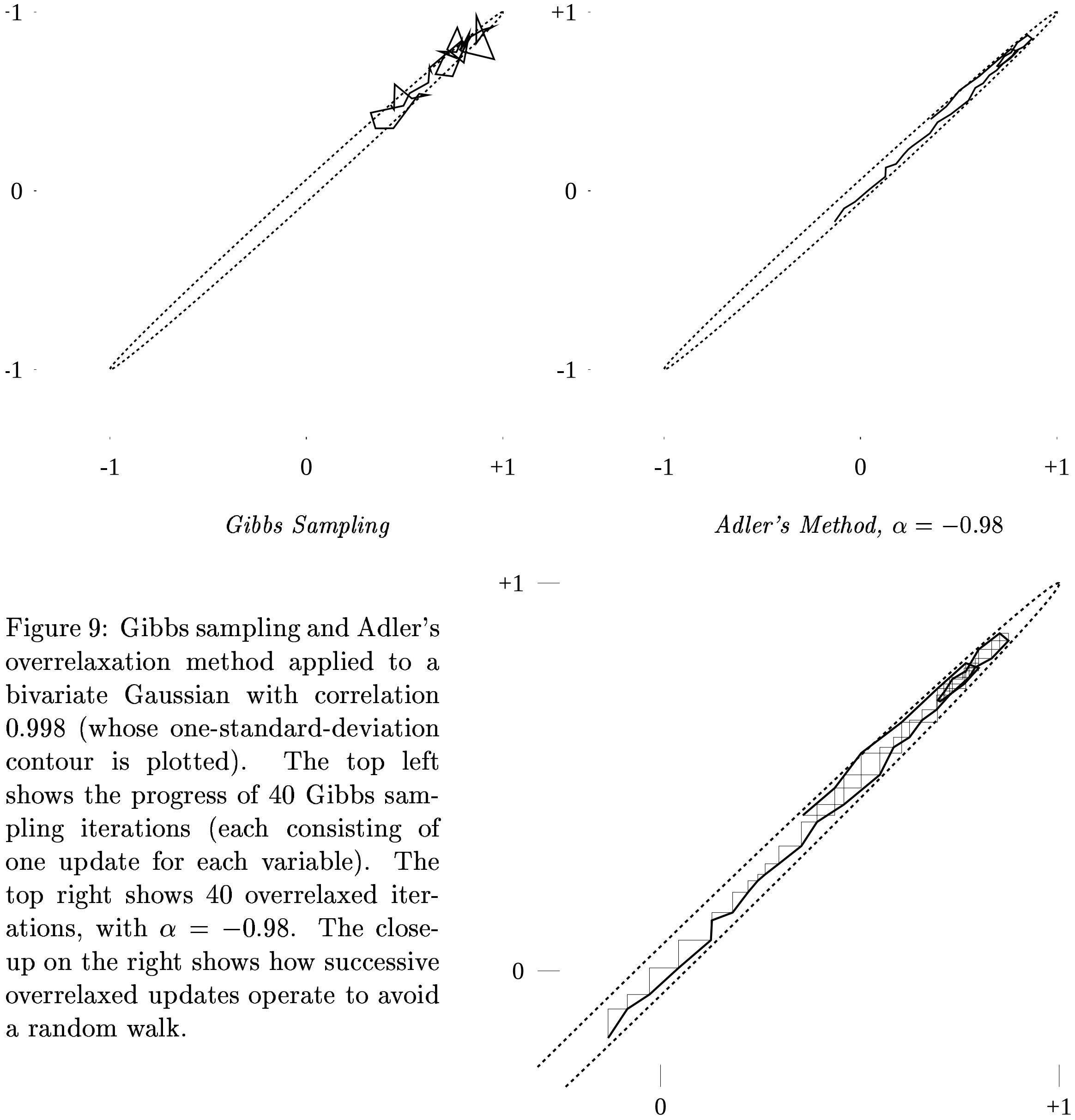
Various attempts have been made to produce overrelaxation schemes that can be used when the conditional distributions are not Gaussian. I have reviewed several such schemes, and introduced one of my own (Neal 1998). The concept of overrelaxation seems to apply only when the conditional distributions are unimodal, so we may assume that this is usually the case, though we would like the method to at least remain valid (ie, leave the desired distribution invariant) even if this assumption turns out to be false. To obtain the full benefits of overrelaxation, it is important that almost every update be overrelaxed, with few or no 'rejections' that leave the state unchanged, as such rejections re-introduce an undesirable random walk aspect to the motion through state space (Neal 1998).

In this section, I will show how overrelaxation can be done using slice sampling. Many schemes for overrelaxed slice sampling are possible, but I will describe only one in detail, based on the stepping out procedure and on bisection. This scheme is illustrated in Figure 10, and given in detail in Figure 11.

To begin, we apply the stepping out procedure of Figure 3 to find an interval around the current point. Normally, we would apply this procedure with the maximum size of the interval (m) set to infinity, or to some large value, since a proper overrelaxation operation requires that the entire slice be found, but the scheme remains valid for any m.

If the stepping out procedure found an interval around the slice that is bigger than the initial interval, then the two outermost steps will serve to locate the endpoints of the slice to within an interval of size w. (Here, we assume that the slice consists of a single interval, as it will if the distribution is unimodal.) We then locate the endpoints more precisely using a bisection procedure. For each endpoint, we test whether the mid-point of the interval within which it is located is inside or outside the slice, and shrink this interval appropriately to narrow the location of the endpoint. This is repeated a times, after which each endpoint will be known to lie within an interval of size $2^{-a}\,w$.

If the stepping out procedure found that the initial interval (of size w) already had both ends outside the slice, then before doing any bisection, we narrow this interval, by shrinking



Gibbs Sampling

Adler's Method, $\alpha = -0.98$

Figure 9: Gibbs sampling and Adler's overrelaxation method applied to a bivariate Gaussian with correlation 0.998 (whose one-standard-deviation contour is plotted). The top left shows the progress of 40 Gibbs sampling iterations (each consisting of one update for each variable). The top right shows 40 overrelaxed iterations, with $\alpha = -0.98$. The close-up on the right shows how successive overrelaxed updates operate to avoid a random walk.

it in half repeatedly until its mid-point is within the slice. We then use bisection as above to locate the endpoints to within an interval of size $2^{-a}\,w$.

Once the locations of the endpoints have been narrowed down, we can approximate the entire slice by the interval $(\hat{L}, \hat{R})$, formed from the outer bounds on the endpoint locations. To do an overrelaxed update, we flip from the current point, x_0, to a new point, x_1, that is the same distance as the current point from the middle of this interval, but on the opposite side. That is, we let

$$x_1 \;\;=\;\; \frac{\hat{L}+\hat{R}}{2} \;-\; \left(x_0 - \frac{\hat{L}+\hat{R}}{2}\right) \;\;=\;\; \hat{L} \;+\; \hat{R} \;-\; x_0 \tag{11}$$

We must sometimes reject this candidate point, in which case the new point is the same as the current point. First of all, we must reject x_1 if it lies outside the interval, $(\bar{L}, \bar{R})$, that had been found prior to bisection, since the interval found from x_1 would then be different, and

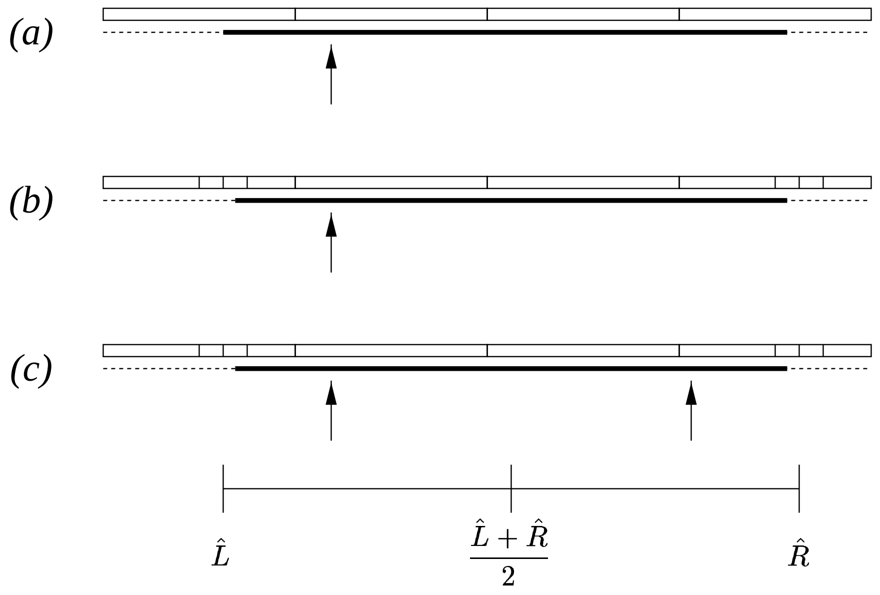


Figure 10: Overrelaxation using the stepping out procedure and bisection. In *(a)*, an interval with both ends outside the slice is found by stepping out from the current point, as was illustrated in Figure 1(b). In *(b)*, the endpoints of the slice are located more accurately using bisection. In *(c)*, a candidate point is found by flipping through the point half-way between the approximations to the endpoints. In this case, the candidate point is accepted, since it is within the slice, and within the orginal interval (prior to bisection).

detailed balance would not hold. However, this situation cannot arise when the distribution is unimodal. Secondly, we must reject x_1 if it lies outside the slice. This can easily happen for a multimodal distribution, and can happen even for a unimodal distribution when the endpoints of the slice have not been located exactly. However, the probability of rejection for a unimodal distribution can be reduced to as low a level as desired, at moderate cost, by locating the endpoints more precisely using more iterations of bisection.

The correctness of this procedure can be seen using arguments similar to those of section 4.3. The interval before bisection can be found by the doubling procedure instead of stepping out, provided the point found is rejected if it fails the acceptance test of Figure 6. However, rejection for this reason will not occur in the presumably typical case of a unimodal distribution.

One could use many methods other than bisection to narrow down the locations of the endpoints before overrelaxing. If the derivative of $f(x)$ can easily be calculated, one could use Newton iteration, whose rapid convergence would often allow the endpoints to be calculated to machine precision in a few iterations. For unimodal distributions, such exact calculations would eliminate the possibility of rejection, and would also make the final result be independent of the way the interval containing the slice was found, thereby allowing use of retrospective methods for tuning the procedure for finding this interval.

To obtain a full sampling scheme, overrelaxed updates of this sort would be applied to each variable in turn, in a fixed order, for a number of cycles, after which a normal slice sampling update would be done. Alternatively, each update could be done normally with

```
Input:   $f$  = function proportional to the density
         $x_0$  = the current point
         $y$  = the vertical level defining the slice
         $w$  = estimate of the typical size of a slice
         $a$  = integer limiting endpoint accuracy to $2^{-a}\,w$
         $(L, R)$  = interval found by the stepping out procedure

Output:  $x_1$  = the new point

$\bar{L} \leftarrow L, \;\; \bar{R} \leftarrow R$
$\bar{w} \leftarrow w, \;\; \bar{a} \leftarrow a$

When the interval is only of size w, the following section will narrow it
until the mid-point is inside the slice (or the accuracy limit is reached).

if $R - L < 1.1 * w$ then
    repeat:
        $M \leftarrow (\bar{L} + \bar{R})\,/\,2$
        if $\bar{a} = 0$ or $y < f(M)$ then exit loop
        if $x_0 > M$ then $\bar{L} \leftarrow M$ else $\bar{R} \leftarrow M$
        $\bar{a} \leftarrow \bar{a} - 1$
        $\bar{w} \leftarrow \bar{w}\,/\,2$

Endpoint locations are now refined by bisection, to the specified accuracy.

$\hat{L} \leftarrow \bar{L}, \;\; \hat{R} \leftarrow \bar{R}$
repeat while $\bar{a} > 0$:
    $\bar{a} \leftarrow \bar{a} - 1$
    $\bar{w} \leftarrow \bar{w}\,/\,2$
    if $y \geq f(\hat{L} + \bar{w})$ then $\hat{L} \leftarrow \hat{L} + \bar{w}$
    if $y \geq f(\hat{R} - \bar{w})$ then $\hat{R} \leftarrow \hat{R} - \bar{w}$

A candidate point is found by flipping from the current point to the
opposite side of $(\hat{L}, \hat{R})$. It is then tested for acceptability.

$x_1 \leftarrow \hat{L} + \hat{R} - x_0$
if $x_1 < \bar{L}$ or $x_1 > \bar{R}$ or $y \geq f(x_1)$ then
    $x_1 \leftarrow x_0$
```

Figure 11: The overrelaxation procedure using bisection. It is assumed that the interval (L, R) was found by the stepping out procedure, with a stepsize of w.

some small probability. A Markov chain consisting solely of overrelaxed updates might not be ergodic, and might in any case suppress random walks for too long. The frequency of normal updates is a tuning parameter, analogous to the choice of α in Adler's overrelaxation method, and would ideally be set so that the Markov chain moves systematically, rather than in a random walk, for long enough that it traverses a distance comparable to the largest dimension of the multivariate distribution, but for no longer than this. To keep from doing a random walk for around k steps, one would do every k'th update normally, and also arrange for the rejection rate for the overrelaxed updates to be less than $1/k$.

7 Reflective slice sampling

Multivariate slice sampling methods can also be designed to suppress random walks. In this section I describe methods that 'reflect' off the boundaries of the slice. Such movement with reflection can be seen as a specialization to uniform distributions of the Hamiltonian dynamics that forms the basis for Hybrid Monte Carlo (Duane, *et al* 1987).

As before, suppose we wish to sample from a distribution over $\Re^n$, defined by a function $f(x)$ that is proportional to the probability density, and which we here assume is differentiable. We must be able to calculate both $f(x)$ and its gradient (or equivalently, the value and gradient of $\log f(x)$). In each iteration of the Markov chain, we will draw a value for an auxiliary variable, y, uniformly from $(0, f(x))$, thereby defining an n-dimensional slice $S = \{\, x \,:\, y < f(x) \,\}$. We will also introduce n additional 'momentum' variables, written as a vector p, which serve to indicate the current direction and speed of motion through state space. At the start of each iteration, we pick a value for p, independently of x, from some rotationally symmetric distribution, typically Gaussian with mean zero and identity covariance matrix.

Once y and p have been drawn, we repeatedly update x by stepping in the direction of p. After some predetermined number of steps, we take the final value of x as our new state (provided it is acceptable). In each step, we try to set $x' = x + wp$, for some scale parameter w that determines the average step size. However, if the resulting x' is outside the slice S (ie, $y \geq f(x')$), we must somehow bring try to bring it back inside. The schemes considered here all do this by some form of reflection, but differ in the exact procedure used.

Ideally, we would reflect from the exact point at which movement in the direction of p first takes us outside the slice. This reflection operation modifies p, after which motion continues in the new direction, until we again encounter the boundary of the slice. When we hit the boundary at a point where the gradient of $f(x)$ is g, reflection will change p as follows:

$$p' \;=\; p \;-\; 2\,g\,\frac{p \cdot g}{|g|^2} \tag{12}$$

This ideal reflection scheme is illustrated for a two-dimensional slice in Figure 12. Using the fact that the reflection transformation above has Jacobian one and is its own inverse, one can show that movement with reflection for some pre-determined duration leaves invariant the joint distribution of x (uniform within the slice) and p (rotationally symmetric, independent of x), so this way of sampling is valid, with no need for an acceptance test. One can also see

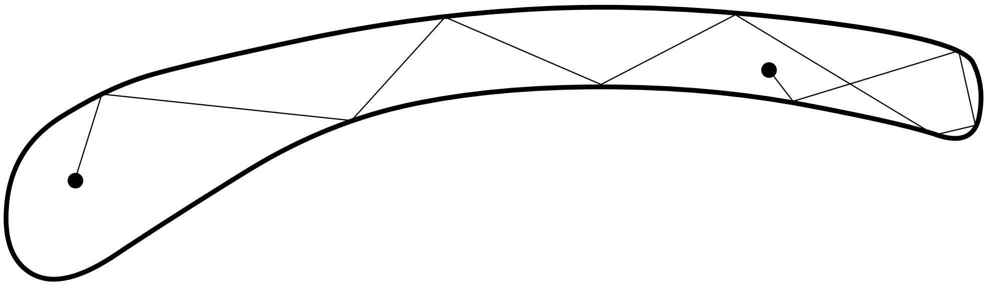


Figure 12: Moving around a two-dimensional slice by reflection from the exact boundaries.

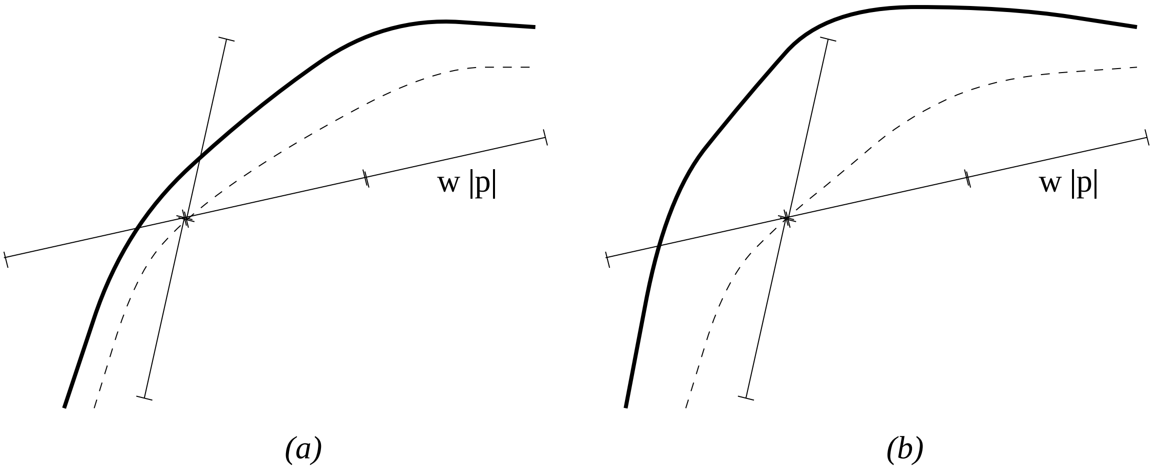


Figure 13: Reflection from an inside point. The trajectories here go in steps of size $w|p|$, starting from the top right, until a point outside the slice is reached, when a reflection is attempted based on the inner contour shown. In *(a)*, the reflection is is sucessful; in *(b)*, it must be rejected, since the reverse trajectory would not reflect at this point.

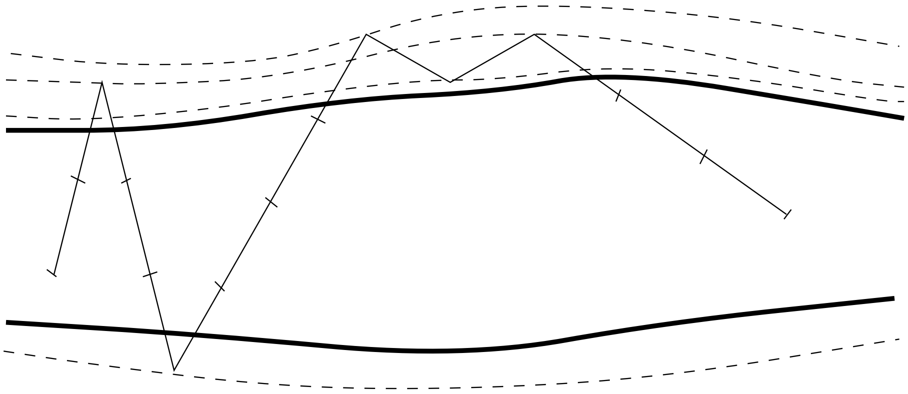


Figure 14: Reflection from outside points. Starting from the left, two reflections based on outside contours lead back inside the slice after the next step. The step after the third reflection is still outside the slice, so further reflections must be done. In this case, the trajectory eventually returns to the slice, and its endpoint would therefore be accepted.

from the figure how such motion can proceed consistently in one direction (until the end of the slice is reached), rather than in a random walk.

Ideal reflection is difficult to implement, however, as it requires precise calculation of where the current path intersects the boundary of the slice. Finding this point analytically might sometimes be possible, or we might try to solve for it numerically, but if the slice is not known to be convex, it may be difficult even to determine with certainty that an intersection point that has been found is in fact the first one that would be encountered. Rather than attempt such exact calculations, we can instead employ one of two approximate schemes, based on 'inside' or 'outside' reflection, although the trajectories these schemes produce must sometimes be rejected.

When stepping from x to $x' = x + wp$ takes us outside the slice, we can try to reflect from the last inside point, x, instead of from the exact point where the path intersects the boundary, using the gradient of $f(x)$ at this inside point. The process is illustrated in Figure 13. However, for this method to be valid, we must check that the reverse trajectory would also reflect at this point, by verifying that a step in the direction opposite to our new heading would take us outside the slice. If this is not so, we must either reject the entire trajectory of which this reflection step forms a part, or alternatively, set p and x so that we retrace the path taken to this point (starting at the inside point where the reflection failed).

Alternatively, when we step outside the slice, we can try to reflect from the outside point, x', based on the gradient at that point. A trajectory with several such reflections is shown in Figure 14. After performing a pre-determined number of steps, we accept the trajectory if the final point is inside the slice. Note that for this method to be valid, one must reflect *whenever* the current point is outside the slice, even if this leads one away from the slice rather than toward it. This will sometimes result in the trajectory never returning to the slice, and hence being rejected, but other times, as in the figure, it does return eventually.

Many variations on these procedures are possible. Above, it was assumed that values for y and p are are randomly drawn at the beginning of a trajectory, and then kept the same for many steps (apart from the changes to p when reflections occur). When using inside reflection, we might instead pick a new value for y more often, perhaps before every step, and we might also partially update p, as is done in Horowitz's (1991) variation on Hybrid Monte Carlo. When using outside reflection, the acceptance rate can be increased by terminating the trajectory when either some pre-set maximum number of steps have been taken, *or* some pre-set number of steps have ended inside the slice. When termination occurs for the latter reason, the final point will necessarily be inside the slice, and the trajectory will therefore be accepted.

8 A Demonstration

To illustrate the benefits stemming from the adaptive nature of slice sampling, I show here how it can help avoid a disastrous scenario, in which a seriously wrong answer is obtained without any obvious indication that something is amiss.

The task is to sample from a distribution for ten real-valued variables, v and x_1 to x_9. The marginal distribution of v is Gaussian with mean zero and standard deviation 3. Conditional on a given value of v, the other variables, x_1 to x_9, are independent, with the conditional distribution for each being Gaussian with mean zero and variance e^v. The resulting shape resembles a ten-dimensional funnel, with small values for v at its narrow end, and large values for v at its wide end. Such a distribution is typical of priors for components of Bayesian hierarchical models — x_1 to x_9 might, for example, be random effects for nine subjects, with v being the log of the variance of these random effects. If the data happens to be largely uninformative, the problem of sampling from the posterior will be similar to that of sampling from the prior, so this test is relevant to actual Bayesian inference problems.

It is of course possible to sample from this distribution directly, by simply sampling for v, and then sampling for each of x_1 to x_9 given this value for v, thereby obtaining independent points from exactly the correct distribution. And in any case, we already know the correct marginal distribution for v, which will be the main focus below. For this test, however, we will pretend that we don't already know the answer, and then compare what we would conclude using various Markov chain methods to what we know is actually correct.

Figure 15 shows the results of trying to sample from this distribution using Metropolis methods. The upper plot shows 2000 iterations of a run in which each iteration consists of 10000 multivariate Metropolis updates (ie, 20 million Metropolis updates altogether). The proposal distribution used was a spherical Gaussian centred on the current state, with standard deviation of one for each of the ten variables. The initial state had $v = 0$ and all $x_i = 1$, which is a typical magnitude for the x_i given that $v = 0$. The points plotted are the value of v at each iteration. Dotted lines are shown at $v = \pm 7.5$.

The results of this run are grossly incorrect. We know that the marginal distribution for v is Gaussian with mean zero and standard deviation 3. One would expect that out of 2000 points from this distribution, on average 95.6 (4.8%) should be less than -5, but none of the points sampled by the multivariate Metropolis method are in this region. Moreover, there is little in the plot to indicate that anything is wrong. In an actual application, the results of a run such as this could easily be accepted as being correct, with serious consequences.

The source of the problem is the low probability of accepting a proposal when in a state where v is small. When v is -4, for example, the standard deviation of the x_i conditional on this value for v is 0.135. The chances that a multivariate Metropolis proposal in which each x_i has standard deviation one will produce values for all the x_i that are within this range of zero is about $0.135^9 \approx 1.5 \times 10^{-8}$. The proposal will include a change to v as well as the x_i, so this calculation does not give the exact acceptance probability, but it does indicate that when v is small, the acceptance probability can become very small, and the chain will remain in the same state for a very long time. Since the Markov chain leaves the correct distribution invariant, it follows that the chain will only very rarely move from a large value of v (which happens to be where this run was started) to a small value for v — indeed, this never occurred in the actual run.

Once one suspects a problem of this sort, signs of it can be seen in the plot. In particular, starting at iteration 1198, the value of v stays at around -3.3 for 25 iterations (ie, for 250,000 Metropolis updates). However, there are no obvious occurrences of this sort in the

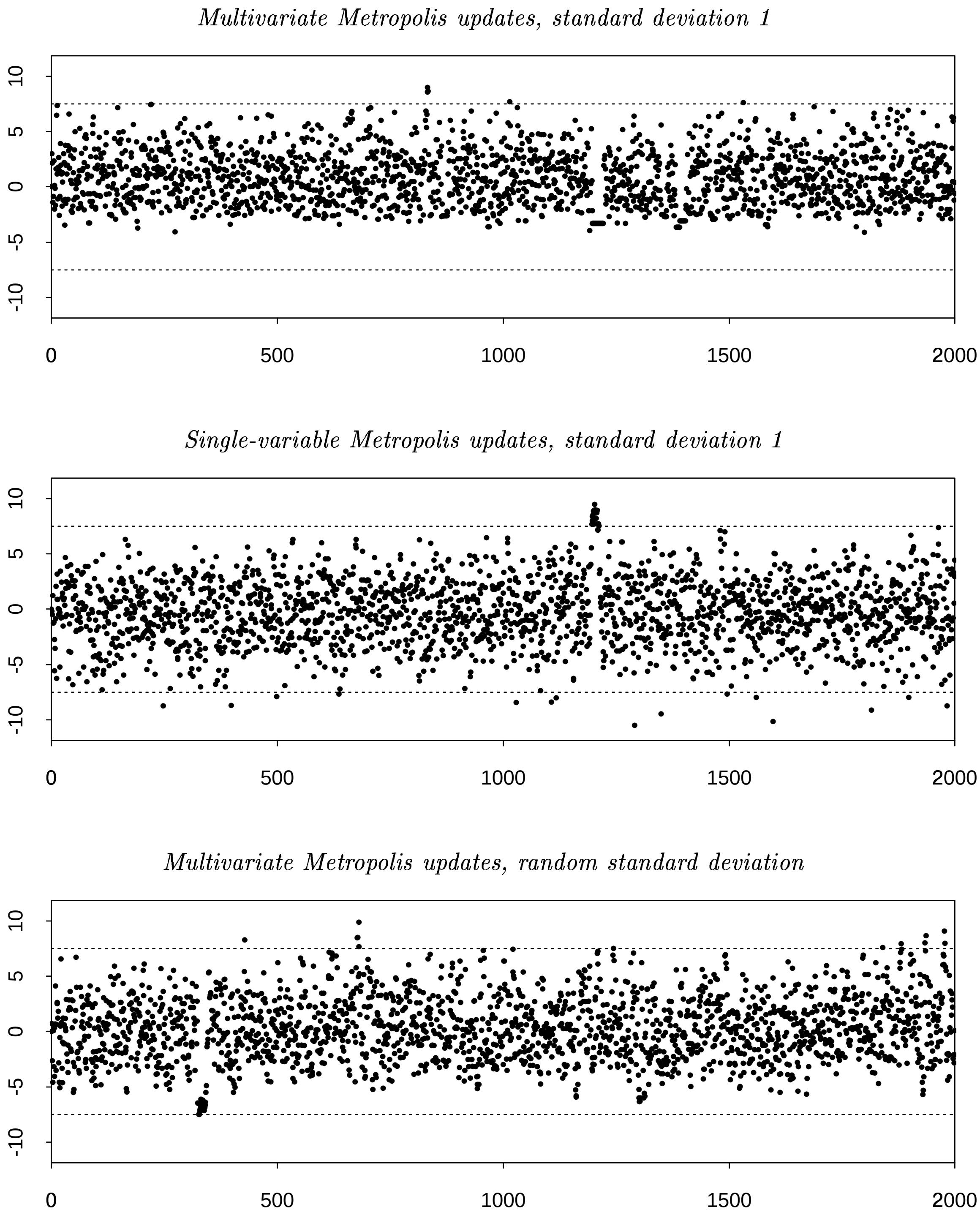


Figure 15: Sampling from the funnel distribution with Metropolis methods.

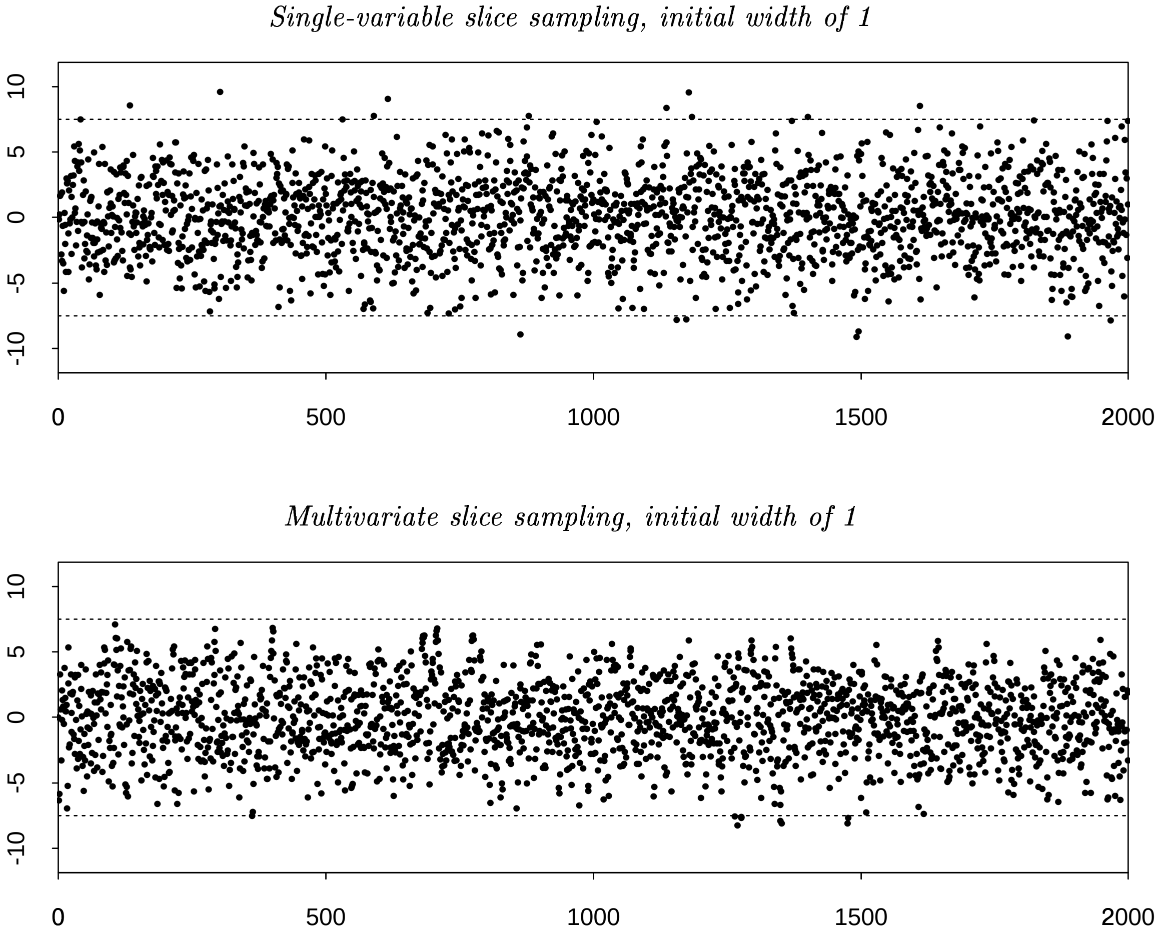
first 1000 iterations, so the problem would not be apparent even to a suspicious user if only half as many iterations had been done. Running several chains from different starting states might have revealed the problem, but when sampling from more complex distributions, it is difficult to be sure that an appropriate variety of starting states has been tried.

The middle plot in Figure 15 shows the results of sampling from the funnel distribution using single-variable Metropolis updates, applied to each variable in sequence. The proposal distribution was a Gaussian centred on the current value, with standard deviation one. Each iteration for this run consisted of 1300 updates for each variable in turn, which take approximately as long as 10000 multivariate Metropolis updates (with the program and machine used). As before, the plot shows the value of v after each of 2000 such iterations.

The results using single-variable Metropolis updates are not as grossly wrong as those obtained using multivariate Metropolis updates. Small values for v are obtained in the expected proportion. The previous problem of very low acceptance rates when v is small is avoided because even when the standard deviation for one of the x_i given v is much smaller than the proposal standard deviation, proposals to change a single x_i are still accepted occasionally (eg, when $v = -9$, the standard deviation of the x_i is 0.011, and about one proposal in 100 is accepted).

However, *large* values for v are sampled poorly in this run. About 0.6% of the values should be greater than 7.5 (which is marked by a dotted line), but no such values are seen in the first half of the run (1000 iterations, 1.3 million updates for each variable). Around iteration 1200, the chain moves to large values of v and stays there for 17 iterations (22100 updates for each variable). This number of points above 7.5 is not too far from the expected number in 2000 iterations, which is 12.4, so in this sense the run produced approximately the right answer. However, it is clear that this was largely a matter of luck. Movement to large values of v is rare, because once such a value for v is reached, the chain is likely to stay at a large value for v for a long time. In this case, the problem is not a high rejection rate, but rather slow exploration of the space in small steps. For example, the standard deviation of the x_i when v is 7.5 is 42.5. Exploring a range of plus or minus twice this by a random walk with steps of size around one takes about $(4 \times 42.5)^2 = 28900$ updates of each variable. While exploring this range, substantial amounts of time will be spent with values for the x_i that are not compatible with smaller values of v. (This problem is not as severe in the previous run, because the multivariate proposals take larger steps, since they change all variables at once.)

We might try to avoid the problems sampling for both large and small values of v by picking the proposal standard deviation at random, from a wide range. The lower plot in Figure 15 shows the results when using multivariate Metropolis proposals in which the log base 10 of the proposal standard deviation is chosen uniformly from the interval $(-3, 3)$. Large values for v are sampled fairly well, but small values for v are still a problem, though the results are not as bad as for multivariate Metropolis with the proposal standard deviation fixed at one. Increasing the range of proposal standard deviations to even more than six orders of magnitude might fix the problem, but at an even greater cost in wasted computation when the random choice is inappropriate.


Single-variable slice sampling, initial width of 1

Multivariate slice sampling, initial width of 1

Figure 16: Sampling from the funnel distribution with slice sampling methods.

Figure 16 shows the results of trying to sample from the funnel distribution using slice sampling methods. In the upper plot, single-variable slice sampling was used, with an initial interval of size one, expanded by the stepping-out procedure (Figure 3) until both ends are outside the slice, and then sampled from with the shrinkage procedure (Figure 5). Each of the 2000 iterations done consisted of 120 such updates for each variable in turn, which takes approximately the same amount of time as the Metropolis methods of Figure 15. The average number of evaluations of f for these slice sampling updates was 12.7, but a few updates required more than a hundred evaluations.

The results with single-variable slice sampling are quite good. Small values of v are perhaps sampled slightly less well than with single-variable Metropolis updates (Figure 15, middle plot), but the difference is not large. Large values of v are sampled better than with any of the Metropolis methods.

The lower plot in Figure 16 shows the results when using the multivariate slice sampling procedure of Figure 8, with an initial hyperrectangle with sides of length one. Sampling is good out to values of v of about ±7.5, but the extreme tails are not sampled well. Recall that this procedure does not expand the initial hyperrectangle, which explains the poor sampling for large values of v. The problem with small values of v is probably due to shrinkage being done for all dimensions of the hyperrectangle, with the result that changes to v are very small when v is small (since changes to the x_i must then be small). As mentioned briefly in Section 5.1, ways to improve the method in both respects could be explored.

9 Discussion

As seen in this paper, the idea of slice sampling can be used to produce many Markov chain sampling schemes. In Figure 17, I attempt to summarize the characteristics of these schemes, and of some competing approaches for sampling from general distributions on continuous state spaces.

The table separates single-variable methods that update each variable in turn from multivariate methods that update all variables at once. Single-variable methods may be preferred

	Derivatives needed?	*How critical is tuning?*	*Retrospective tuning allowed?*	*Can suppress random walks?*
Single-variable methods				
ARS/ARMS	No (but helpful)	Low/Medium	If log concave	No
Single-variable Metropolis	No	Medium	No	No
Single-variable slice sampling	No	Low	If unimodal	No
Overrelaxed slice sampling	No (but helpful)	Low	If unimodal and endpoints exact	Yes
Multivariate methods				
Multivariate Metropolis	No	Medium-High	No	No
Dynamical methods	Yes	High	No	Yes
Slice sampling with hyperrectangles	No	Low–Medium	No	No
Slice sampling with Gaussian crumbs	Possibly helpful	Low–Medium	No	No
Reflective slice sampling	Yes	Medium–High	No	Yes

Figure 17: Characteristics of some general-purpose Markov chain sampling methods.

when the coordinate system used is such that one expects many of the variables to be almost independent, allowing these variables to change by a large amount even when the other variables are fixed. Also, for some models, recomputing the probability density after a change to one variable may be much faster than recomputing it after a change to all variables. On the other hand, if there are strong dependencies between variables, using single-variable updates may lead to slow convergence, or even a lack of ergodicity — though for high-dimensional problems with strong dependencies, simple-minded multivariate methods will also be quite slow.

The first column in the table indicates whether the method requires that derivatives of the (unnormalized) probability density be computable. Derivatives are needed by dynamical methods and reflective slice sampling, which limits their applicability. Adaptive rejection sampling (Gilks and Wild 1992; Gilks 1992) and overrelaxed slice sampling can take advantage of derivatives, but can operate without such information with only a moderate loss of efficiency — eg, when no derivatives are available, overrelaxed slice sampling can use bisection rather than Newton iteration to find the endpoints of the slice.

The second and third columns indicate how critical it is that tuning parameters be set to good values, and whether or under what conditions 'retrospective tuning' is allowed — that is, whether parameters of the method can be set based on information from past iterations. Adaptive rejection sampling (ARS) for log concave distributions is very good in these respects — a parameter is needed for the size of the first step taken in search of a point on the other size of the mode, but subsequent steps can be made larger (eg, by doubling), so the effect of a poor initial step is not too serious; furthermore, it is allowable to set this size parameter based on the stepsize that was found to be necessary in previous iterations. Parameter tuning is more of a problem when ARMS (Gilks, Best, and Tan 1995) is used for distributions not known to be log concave — a poor choice of parameters may have worse effects, and retrospective tuning is not allowed (Gilks, Neal, Best, and Tan 1997). Tuning is also a problem for single-variable and multivariate Metropolis methods — proposing changes that are too small leads to an inefficient random walk, while proposing changes that are too large leads to frequent rejections. Using too small a stepsize with a dynamical method is not quite as bad, since movement is not in a random walk, but too large a stepsize is disastrous, since the dynamical simulation becomes unstable, and very few changes are accepted. For Metropolis and dynamical methods, the stepsize parameter must not be set retrospectively.

Single-variable slice sampling and overrelaxed slice sampling offer advantages over other methods in these respects. Whereas ARS/ARMS allows retrospective tuning only for log concave distributions, this is allowed for these slice sampling methods when they are applied to any unimodal distribution (provided the interval is expanded to the whole slice, and endpoints for overrelaxation are computed exactly). Furthermore, the tuning is less critical for slice sampling than for the other methods (apart from ARS), as discussed further below. For reflective slice sampling, however, tuning is at least moderately critical, though perhaps less so than for dynamical methods, and retrospective tuning is not allowed. Tuning for multivariate slice sampling using hyperrectangles is less critical than for multivariate Metropolis methods, but as was seen in the demonstration of Section 8, tuning can be more critical for multivariate slice sampling than for single-variable slice sampling.

The final column indicates whether the method can potentially suppress random walk behaviour. This is important when sampling from a distribution with high dependencies between variables, as in such a situation, exploration of the distribution may have to proceed in small steps, and the difference in efficiency between diffusive and systematic exploration of the distribution can be very large (as is typical, for example, with neural network models (Neal 1996)).

Another way of exploring the differences between these methods is to see how well they work in various circumstances. The most favourable situation is when our prior knowledge lets us choose good tuning parameters for all the methods (eg, the width of a Metropolis proposal distribution or of the initial interval for slice sampling). A Metropolis algorithm with a simple proposal distribution will then move about the distribution fairly efficiently (although in a random walk), and will have low overhead, since it requires evaluation of $f(x)$ at only a single new point in each iteration. Single-variable slice sampling will be comparably efficient, however, provided we stick with the interval chosen initially (ie, we set $m = 1$ in the stepping out procedure of Figure 3). There will then be no need to evaluate $f(x)$ at the boundaries of the interval, and if the first point chosen from this interval is within the slice, only a single evaluation of $f(x)$ will be done. If this point is outside the slice, further evaluations will be required, but this inefficiency corresponds to the possibility of rejection with the Metropolis algorithm. This situation is similar for multivariate slice sampling with an initial hyperrectangle that is not expanded. Metropolis and slice sampling methods should therefore perform quite similarly. However, slice sampling will work better if it turns out that we mistakenly chose too large a width for the Metropolis proposal distribution and the initial slice sampling interval. This error will lead to a high rejection rate for the Metropolis algorithm, but the sampling procedures of Figures 5 and 8 use the rejected points to shrink the interval, which is much more efficient when the initial interval was too large.

As seen in the demonstration of Section 8, the advantage of slice sampling over Metropolis methods can be quite dramatic if we don't know enough to choose a good tuning parameter, or if no single value of the tuning parameter is appropriate for the entire distribution.

Another possibility is that we know that the conditional distributions are log concave, but we do not know how wide they are. Adaptive Rejection Sampling (ARS) then works very well, because its width parameter can be retrospectively tuned, based on previous iterations. Single-variable slice sampling will also work well, since in this situation it can also be tuned retrospectively (provided no limit is set on the size of the interval). However, ARS does true Gibbs sampling, whereas the slice sampling updates do not produce points that are independent of the previous point. Such dependency is probably a disadvantage (unless deliberately directed to useful ends, as in overrelaxation), so ARS is probably better than single-variable slice sampling in this context.

Suppose, however, that we know only that the conditional distributions are unimodal, but not necessarily log concave. We would then need to use ARMS rather than ARS, and would not be able to tune it retrospectively, whereas we can still use single-variable slice sampling with retrospective tuning. This will likely not be as good as true Gibbs sampling, however, which we should prefer if the conditional distribution happens to be one that can be efficiently sampled from. In particular, if slice sampling is used to sample from a heavy-tailed distribution, it may move only infrequently between the tails and the central region, since this transition can occur only when we move to a point under the curve of $f(x)$ that is as low as the region under the tails, but whose horizontal position is in the central region. However, there appears to be no general purpose scheme that avoids problems in this situation.

Finally, consider a situation where we do not know that the conditional distributions are unimodal, and have only a rough idea of an appropriate width parameter for a proposal distribution or initial slice sampling interval. Single-variable slice sampling copes fairly well with this uncertainty. If the initial interval is too small it can be expanded as needed, either by stepping out or by doubling (which is better will depend on whether the faster expansion of doubling is worth the extra overhead from the acceptance test of Figure 6). If instead the initial interval is too big, it will be shrunk efficiently by the procedure of Figure 5. We might try to achieve similar robustness with the Metropolis algorithm by doing several updates for each variable, using proposal distributions with a range of widths. For example, if w is our best guess at an appropriate width, we might do updates with widths of $w/4$, $w/2$, w, $2w$, and $4w$. This may ensure that an appropriate proposal distribution is used some of the time, but it is unattractive for two reasons. First, the limits of the range (eg, from $w/4$ to $4w$) must be set *a priori*. Second, for this approach to be valid, we must continue through the original sequence of widths even after it is clear that we have gone past the appropriate one. These problems are not present with slice sampling.

In any of these situations, we might prefer to use a method that can suppress random walks. Dynamical methods such as Hybrid Monte Carlo (Duane, *et al* 1987) do this well for a wide range of distributions; reflective slice sampling may also work for a wide range of distributions, but preliminary indications are that is less efficient than Hybrid Monte Carlo, when both are tuned optimally. Overrelaxation is sometimes beneficial, but not always (whether it is or not depends on the types of correlation present). For problems where overrelaxation is helpful, overrelaxed slice sampling may often be the best approach to suppressing random walks. If the conditional distributions are unimodal, it offers the possibility of retrospective tuning. It does not require computation of derivatives. For some models, the fact that overrelaxation updates one variable at a time will permit computational saving, in comparison with the simultaneous updates for dynamical and reflective methods.

Multivariate slice sampling using hyperrectangles does not appear to offer much, if any, advantage over single-variable slice sampling, except for the uncommon situation were it is known that the coordinate system used is especially bad (and hence updating variables singly will be particularly inefficient). However, the more general framework for multivariate slice sampling based on 'crumbs' that was outlined in Section 5.2 offers the possibility of adapting not just to the scales of the variables, but also to the dependencies between them. The benefits of such methods can only be determined after further research, but huge increases in efficiency would seem conceivable, if one is to judge from the analogous comparison of minimization by simple steepest descent versus more sophisticated quasi-Newton or conjugate gradient methods.

The practical utility of the slice sampling methods described here will ultimately be determined by experience on a variety of applications. Some such applications will involve tailor-made sampling schemes for particular models — for instance, Frey (1997) used slice sampling successfully to sample for latent variables in a neural network. Slice sampling is also particularly suitable for use in automatically generated samplers, and is now used in some situations by the WinBUGS system (Lunn, *et al* 2000). Readers can try out slice sampling methods for themselves, on a variety of Bayesian models, using the "software for flexible Bayesian modeling" that is available from my web page. This software (version of 2000-08-21) implements most of the methods discussed in this paper.

Acknowledgements

I thank Brendan Frey, Gareth Roberts, Jeffrey Rosenthal, and David MacKay for helpful discussions. This research was supported by the Natural Sciences and Engineering Research Council of Canada and by the Institute for Robotics and Intelligent Systems.

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