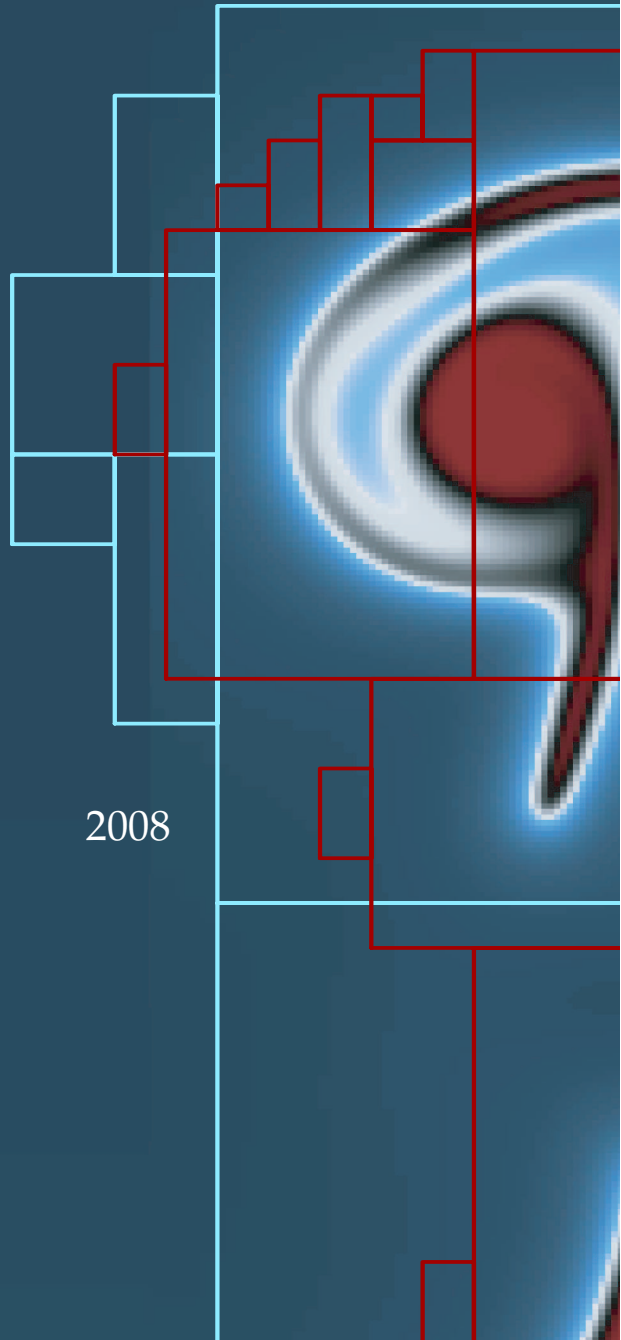


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**MONTE CARLO WITHOUT CHAINS**

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## MONTE CARLO WITHOUT CHAINS

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A sampling method for spin systems is presented. The spin lattice is written as the union of a nested sequence of sublattices, all but the last with conditionally independent spins, which are sampled in succession using their marginals. The marginals are computed concurrently by a fast algorithm; errors in the evaluation of the marginals are offset by weights. There are no Markov chains and each sample is independent of the previous ones; the cost of a sample is proportional to the number of spins (but the number of samples needed for good statistics may grow with array size). The examples include the Edwards–Anderson spin glass in three dimensions.

### 1. Introduction

Monte Carlo sampling in physics is synonymous with Markov chain Monte Carlo (MCMC) for good reasons which are too well-known to need repeating (see for example [3; 17]). Yet there are problems where the free energy landscape exhibits multiple minima and the number of MCMC steps needed to produce an independent sample is huge; this happens for example in spin glass models (see for example [13; 16]). It is therefore worthwhile to consider alternatives, and the purpose of the present paper is to propose one.

An overview of the proposal is as follows: Consider a set of variables (“spins”) located at the nodes of a lattice  $L$  with a probability density  $P$  that one wishes to sample. Suppose one can construct a nested sequence of subsets

$$L_0 \supset L_1 \supset \cdots \supset L_n$$

with the following properties:  $L_0 = L$ ;  $L_n$  contains few points; the marginal density of the variables in each  $L_i$  is known and given values of the spins in  $L_{i+1}$ , the remaining variables in  $L_i$  are independent. Then the following is an effective sampling strategy for the spins in  $L$ : First sample the spins in  $L_n$  so that each configuration is sampled with a frequency equal to its probability (for example, by

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first listing all the states of  $L_n$  and calculating their probabilities). Then sample the variables in each  $L_{i-1}$  as  $i$  decreases from  $n-1$  to zero using the independence of these variables, making sure that each state is visited with a frequency equal to its probability. As a result, each state of  $L = L_0$  is sampled with a frequency equal to its probability, achieving importance sampling; the cost of each sample of  $L$  is proportional to the number of spins in  $L$ , and two successive samples are independent. This can be done exactly in a few uninteresting cases (for example in the one-dimensional Ising model, see for example [15]), but we will show that it can often be done approximately. The errors that come from the approximation can then be compensated for through the use of sampling weights. The examples shown below include spin glass models.

The heart of the construction is the fast evaluation of marginals, of which a previous version was presented in [9]; this is the subject of Section 2. An example of the nested sets needed in the construction above is presented in Section 3. The construction is in general approximate, and the resulting errors are to be compensated for by weights, whose calculation is explained in Section 4; efficiency demands a balance between the accuracy of the marginalization and the variability of the weights, as explained in Sections 4 and 6. The fast evaluation of marginals requires a sampling algorithm but the sampling algorithm is defined only once the marginalization is in place; this conundrum is resolved by an iteration which is presented in Section 5; two iteration steps turn out to be sufficient.

The algorithm is applied to the two-dimensional Ising model in Section 6; this is a check of self-consistency. Aspects of the Edwards–Anderson (EA) spin glass model in three dimensions are discussed in Section 7. Extensions and conclusions are presented in a concluding section (Section 8).

A Monte Carlo scheme without chains for spin systems has been previously considered in [6], and used to examine the neighborhood of a critical point in [20]. The construction of marginals explained below and in the earlier paper [9] is a renormalization in the sense of Kadanoff (more precisely, a decimation) [15]; renormalization has been used by many authors as a tool for speeding up MCMC; see for example [2; 6; 14]. A construction conceptually related to the one here and also based on marginalization, but with a Markov chain, was presented in [25]. An alternative construction of marginals can be found in [21]. There is some kinship between the construction here and the decimation and message passing constructions in [7; 12]. The specific connection between marginalization and conditional expectation used here originated in work on system reduction in the framework of optimal prediction; see [11; 10].

The results in this paper are preliminary in the sense that the marginalization is performed in the simplest way I could imagine; more sophisticated versions are suggested in the results and conclusion sections. Real-space renormalization or

decimation and the evaluation of marginals are one and the same, and the present work could be written in either physics or probability language; it is the second option that has been adopted.

All the examples below are of spin systems with two-valued spins and near-neighbor interactions in either a square lattice in two dimensions or a cubic lattice in three dimensions. The Hamiltonians have the form

$$H = - \sum s_{i,j,k} \sum' J_{i,j,k,\ell} s_{i',j',k'}$$

(with one subscript less in two dimensions); the indices  $i, j, k$  parametrize spatial directions, and the index  $\ell$  parametrizes the direction of the interaction, so that the spin at  $i, j, k$  can have a different interaction with the spin at, say,  $i + 1, j, k$ , than with the spin at  $i, j + 1, k$ . In the Ising case,  $J_{i,j,k,\ell}$  are independent of the indices; in the spin glass case,  $J_{i,j,k,\ell}$  are independent random variables.

## 2. Fast evaluation of approximate marginals

In this section we present an algorithm for the evaluation of marginals, which is an updated version of the algorithm presented in [9]. For simplicity, we assume in this section, as in [9], that the spins live on a two-dimensional lattice with periodic boundary conditions (the generalization to three dimensions is straightforward except for the geometrical issues discussed in Section 3). We show how to go from  $L_0$ , the set of spins at the points  $(i, j)$  of a regular lattice whose probability density is known, to  $L_1$ , the set of spins at the points such that  $(i + j)$  is even, and whose marginal is sought. The probability density function (pdf) of the variables in  $L_1$  can be written in the form  $P_0 = e^{W^{(0)}}/Z$ , where  $W^{(0)} = -\beta H$ ,  $\beta$  is the inverse temperature,  $Z$  is the normalization constant, and the Hamiltonian  $H$  has the form specified in Section 1. To simplify notations, write  $\tilde{J}_{i,j,\ell} = -\beta J_{i,j,\ell}$  and then drop the tildes, so that

$$W^{(0)} = \sum s_{i,j} (J_{i,j,1} s_{i+1,j} + J_{i,j,2} s_{i,j+1}). \quad (2-1)$$

The  $s_{i,j}$  take the values  $\pm 1$ .

Let the marginal density of the spins in  $L_1$  be  $P_1$ . One can always write  $P_1 = e^{W^{(1)}}/Z$ , where  $Z$  is the same constant as in the pdf  $P_0$ . Let  $\hat{S}$  denote the set of spins in  $L_1$ , and  $\tilde{S}$  the set of spins in  $L_0$  but not in  $L_1$ , so that  $S = \hat{S} \cup \tilde{S}$  is the set of spins in  $L_0$ . By definition of a marginal,

$$P_1(\hat{S}) = e^{W^{(1)}} = \sum_{\tilde{S}} e^{W^{(0)}(S)}$$

or

$$W^{(1)} = \log \sum_{\tilde{S}} e^{W^{(0)}(S)}, \quad (2-2)$$

where the summation is over all the values of the spins in  $\tilde{S}$ . Extend the range of values of the spins in  $\hat{S}$  (but not  $\tilde{S}$ ) to the interval  $[0, 1]$  as continuous variables but leave the expression for the Hamiltonian unchanged (this device is due to Okunev [19] and replaces the more awkward construction in [9]). Differentiate (2-2) with respect to one of the newly continuous variables  $s = s_{i,j}$  (we omit the indices  $(i, j)$  to make the formulas easier to read):

$$\frac{\partial W^{(1)}}{\partial s} = W^{(1)'} = \frac{\sum_{\tilde{S}} \frac{\partial W^{(0)}}{\partial s} e^{W^{(0)}(S)}}{\sum_{\tilde{S}} e^{W^{(0)}(S)}},$$

or

$$\frac{\partial W^{(1)}}{\partial s} = E\left[\frac{\partial W^{(0)}}{\partial s} \mid \hat{S}\right],$$

where  $E[\cdot \mid \hat{S}]$  denotes a conditional expectation given  $\hat{S}$ . A conditional expectation given  $\hat{S}$  is an orthogonal projection onto the space of functions of  $\hat{S}$ , and we approximate it by projecting onto the span of a finite basis of functions of  $\hat{S}$ .

Before carrying out this projection, one should note the following properties of  $W^{(1)'} = \frac{\partial W^{(1)}}{\partial s}$ : Take two groups of spins distant from each other in space, say  $S_1$  and  $S_2$ . The variables in these groups should be approximately independent of each other, so that their joint pdf is approximately the product of their separate pdfs. The logarithm of their joint pdf is approximately the sum of the logarithms of their separate pdfs, and the derivative of that logarithm with respect to a variable in  $S_1$  should not be a function of the variables in  $S_2$ . As a result, if one expands  $\frac{\partial W}{\partial s}$  at  $s = s_{i,j}$  for some specific values of  $i$  and  $j$ , one needs only to project on a set of functions of  $s_{i,j}$  and of a few neighbors of the point  $(i, j)$ . It is this observation that makes the algorithm in the present section effective, and it is implied in the Kadanoff construction of a renormalized Hamiltonian; see for example [15].

As a basis on which to project, consider, following Kadanoff, the polynomials in  $\hat{S}$  of the form

$$\psi_{p,q} = \sum_{i,j} s_{i,j} s_{i+p,j+q}$$

for various values of  $p, q$ , as well as polynomials of higher degree in the variables  $\hat{S}$ . Define  $\psi'_{p,q} = \partial \psi_{p,q} / \partial s_{i,j}$ ; the functions  $\psi'_{p,q}$  involve only near neighbors of  $s_{i,j}$  (for example, if  $\psi'_{1,1} = \sum_{\ell,k} s_{\ell,k} s_{\ell+1,k+1}$ , then

$$\psi'_{1,1} = 2(s_{i+1,j+1} + s_{i-1,j-1})$$

(no summation)). Write the approximate conditional expectation of  $W^{(1)'}$  as a sum

$$E[W^{(1)'} \mid \hat{S}] = \sum a_{p,q} \psi'_{p,q} + \dots \quad (2-3)$$

Each function  $\psi_{p,q}$  embodies an interaction, or linkage, between spins  $(p, q)$  apart, and this is an expansion in “successive linkages”. The functions  $W^{(0)}$ ,  $W^{(1)}$  are

invariant under the global symmetry  $s \rightarrow -s$ , and only polynomials having this symmetry need to be considered (but see the discussion of symmetry breaking in Section 6). For the reasons stated above, this series should converge rapidly as  $p, q$  increase. Evaluate the coefficients in (2-3) by orthogonal projection onto the span of the  $\psi'_{p,q}$ . This produces one equation per point  $(i, j)$  (unless the system is translation invariant, like the Ising model, in which case all these equations are translates of each other). Assume furthermore that one has an algorithm for sampling the pdf  $P_0 = e^{W^{(0)}}/Z$  (this is not trivial as the goal of the whole exercise is to find good ways to sample  $P_0$ ; see Section 5). The projection can then be carried out by the usual method: reindex the basis functions with a single integer, so that they become  $\psi_1, \psi_2, \dots$ , say  $\psi_1 = \psi_{1,1}$  and so on; at each point  $(i, j)$  estimate by Monte Carlo the entries  $a_{p,q} = E[\psi_p \psi_q]$  of a matrix  $A$ , and the entries  $b_p = E[W^{(0)'} \psi_p]$  of a vector  $b$ , where  $E[\cdot]$  denotes an expectation. The projection we want is  $\sum a_p \psi'_p$ , where the coefficients  $a_p$  are the entries of the vector  $A^{-1}b$  (see for example [10]). In the current paper we use only the simplest basis with  $\psi_{1,1}, \psi_{1,-1}, \psi_{-1,1}, \psi_{-1,-1}$  (functions such as  $\psi_{0,1}$  or  $\psi_{1,0}$  do not appear because they involve spins not in  $\hat{S}$ ). In three dimensions also we use basis functions of the form  $\sum s_{i,jk} s_{i',j',k'}$  where  $(i', j', k')$  is a near neighbor of  $(i, j, k)$  on a reduced lattice. The locality of the functions  $\psi'$  makes the algorithm efficient; more elaborate basis for the Ising case can be found in [9] and in Section 6 below. We have not invoked here any translation invariance, in view of later applications to spin glasses. For the Hamiltonian (2-1), the quantity  $W^{(0)'} = \frac{\partial W^{(0)}}{\partial s}$  for  $s = s_{i,j}$  is

$$\left. \frac{\partial W^{(0)}}{\partial s} \right|_{i,j} = J_{i,j,1} s_{i+1,j} + J_{i-1,j,1} s_{i-1,j} + J_{i,j,2} s_{i,j+1} + J_{i,j-1,2} s_{i,j-1}.$$

The marginal density of the variables in  $L_2$  (the set of points  $(i, j)$  such that both  $i$  and  $j$  are odd) is obtained by projecting on the basis functions  $\psi_{0,2}, \psi_{0,-2}, \psi_{2,0}, \psi_{-2,0}$  and others. A single sample of all the spins in  $L_0$  can be used to generate samples of the inner products needed to find the coefficients in the projections on all the sublattices; it is not a good idea to use the marginal of  $L_1$  to evaluate the marginal of  $L_2$ , and others, because this may lead to a catastrophic error accumulation [9; 23]; it is the original  $W^{(0)'} = \frac{\partial W^{(0)}}{\partial s}$  that is projected in the expansions at the different levels.

The last step is to reconstruct  $W^{(1)}$  from its derivatives  $W^{(1)'}$ . In the Ising (translation invariant) case, this is trivial:  $W^{(1)'} = \sum a_p \psi'_p$  implies  $W^{(1)} = \sum a_p \psi_p$ . In the spin glass case, there is a minor conceptual (thought not practical) difficulty. For the various functions  $W^{(1)'}$  computed at many points  $(i, j)$  to be derivatives of a single function  $W^{(1)}$  the cross derivatives must be equal. However, this equality requires equalities between expansion coefficients evaluated at different points  $(i, j)$  of the lattice. For example, if  $\psi_1$  after renumbering is  $\psi_{1,1}$  before the renumbering in

the notations above, and  $\psi_3$  is  $\psi_{-1,-1}$  before the renumbering, then the coefficient  $a_3$  at the point  $(i, j)$  should equal the coefficient  $a_1$  at the point  $(i - 1, j - 1)$ , and indeed these coefficients describe the same interaction between the spins at  $(i, j)$  and  $(i - 1, j - 1)$ . However, these coefficients are computed separately by approximate computations, and therefore, though closely correlated (with a correlation coefficient typically above .95), they are not identical. This is not a practical difficulty, because the replacement of one of these coefficients by the other, or of both by some convex linear combination of the two, does not measurably affect the outcome of the calculation. The conceptual issue is resolved if one notices that (i) for every lattice  $L_j$ , except the smallest one  $L_n$ , one needs the coefficients  $a_p$  at only half the points, and using the coefficients calculated at these points is unambiguous, and (ii) allowing these coefficients to differ is the same as writing the Hamiltonian  $W$  as  $(s, Ms)$  where  $s$  is the vector of spins and  $M$  is an asymmetric matrix. However, the values of  $W$  are the same if  $M$  is replaced by its symmetric part, which means replacing each of the two values of a coefficient by the mean of the two values. If this is done everywhere the cross derivatives become equal.

Finally, a practical comment: One may worry about a possible loss of accuracy due to the ill-conditioning of a projection on a nonorthogonal polynomial basis. I did develop an approximate Monte Carlo Gram–Schmidt orthogonalization algorithm in which polynomials approximately orthogonal with respect to the probability density at each level were created by a Monte Carlo process and then projected on; the results did not differ measurably from the results in the present paper. A detailed description of this Gram–Schmidt process will be given in a subsequent paper if its use ever turns out to be worthwhile.

### 3. The nested sublattices

In this section we construct the nested sequence of sublattices  $L = L_0, L_1, \dots$  such that the spins in  $L_j$  are independent once those in  $L_{j+1}$  are determined. There is nothing unique about this construction; the nested sequence should have appropriate independence and approximation properties while leading to efficient programs.

The two-dimensional case was already discussed in the previous section: assume  $L = L_0$  is the set of nodes  $(i, j)$ , with  $i, j$  integers. We can choose as the next smaller array of spins  $L_1$  the set of spins at the location  $(i, j)$  with  $i + j$  even; then the spins in  $L_0$  are independent once in  $L_1$  are known. The next lattice  $L_2$  is the one where  $i, j$  are both odd; if the marginal on  $L_1$  is approximated with the four basis functions described in the previous section, then the spins in  $L_1$  are independent once those in  $L_2$  are given. From then on the subsets  $L_i$  can be constructed by similarity. If periodic boundary conditions are imposed on  $L_0$ , they are inherited by every successive sublattice.



If one wants to carry out an expansion in a basis with more polynomials, the requirement that the spins in  $L_i$  be independent once those in  $L_{i+1}$  are known places restrictions on the polynomials one can use; for example, the polynomial

$$\sum s_{i,j} s_{i+2,j}$$

for  $i, j$  such that  $i + j$  is even is a function of only the spins in  $L_1$  but it cannot be used, because the spins at points where  $i + j$  is even while each of  $i, j$  is odd would not be independent once the spins in  $L_2$  are known, given the linkage created by this added polynomial. This places a restriction on the accuracy of the various marginals; see also the discussion in Section 6. However, the point made in the present paper is that significant inaccuracy in the marginals can be tolerated.

The analogous construction in three dimensions is neither so simple nor unique. Here is what is done in the present paper:  $L_0 = L$  consists of all the nodes on a regular cubic lattice, that is, the set of points  $(i, j, k)$  where  $i, j, k$  are integers between 1 and  $N$  and  $N$  is a power of 2.

$L_1$  consists of the points  $(i, j, k)$  where  $i + j$  is even for  $k$  odd and odd when  $k$  is even; the neighbors of  $(i, j, k)$  in  $L_1$  are the 8 points  $(i, j \pm 1, k \pm 1), (i \pm 1, j \pm 1, k)$ .

$L_2$  consists of the points  $(i, j, k)$  where  $i$  is even,  $j$  is odd and  $k$  is even. The neighbors of a point  $(i, j, k)$  in  $L_2$  are the 12 points  $(i \pm 1, j, k \pm 1), (i \pm 1, j \pm 2, k \pm 1)$ .

$L_3$  consists of the points  $(i, j, k)$  where  $i, j, k$  are all odd; the neighbors of  $(i, j, k)$  are  $(i \pm 2, j, k), (i, j \pm 2, k), (i, j, k \pm 2)$ . This sublattice is similar to the original lattice with the distance between sites increased to 2; the next lattices up can then be obtained by similarity.

This process of constructing sublattices with ever smaller numbers of spins stops when one reaches a number of spins small enough to be sampled directly, that is, by listing all the states, evaluating their probabilities, and picking a state with a frequency equal to its probability. One has to decide what the smallest lattice is; the best one could do in this sequence is a lattice similar to  $L_2$  with the points  $(i, j, k)$  where  $i - 1 = 2\ell, j - 1 = 2\ell$ , and  $k = 2\ell$  for an integer  $\ell$  chosen so that there are 16 points in this smallest lattice. Here too each lattice inherits periodic boundary conditions from the original lattice; on the smallest lattice one notes that due to periodicity  $i + 2\ell = i - 2\ell \pmod{N}$  so that some of the neighbors of a points  $(i, j, k)$  are not distinct and this must be reflected in the evaluation of the last Hamiltonian, or else all the linear systems one solves in the last projection step are singular.

The polynomial basis used in this paper, except in the diagnostics sections, consists at every level of polynomials of the form  $\psi_m = \sum s_{i,j,k} s_{i_m, j_m, k_m}$ , where  $(i, j, k)$  is a point in the sublattice  $L_m$  and  $(i_m, j_m, k_m)$  is one of its near neighbors on that sublattice.

#### 4. Sampling strategy and weights

If the marginals whose computation has just been described were exact, the algorithm outlined in the introduction would be exact. However, the marginals are usually only approximate, and one has to take into account the errors in them, due to both the use of too few basis functions and the errors in the numerical determination of the projection coefficients. The idea here is to compensate for these errors through appropriate weights.

Suppose one wants to compute the average of a function  $h(S)$  of a random variable  $S$ , whose pdf is  $P(x)$ , that is, to compute

$$E[f(S)] = \int h(x)P(x)dx.$$

Suppose one has no way to sample  $S$  but one can sample a nearby variable  $S_0$  whose pdf is  $P_0(x)$ . One then writes

$$\begin{aligned} \int h(x)P(x)dx &= \int h(x)\frac{P(x)}{P_0(x)}P_0(x)dx \\ &= E\left[h(S_0)\frac{P(S_0)}{P_0(S_0)}\right] \cong \frac{1}{Z_s} \sum h(S_{0i})w_i, \end{aligned}$$

where the  $S_{0i}$  are successive samples of  $S_0$ , for  $i = 1, \dots, N_s$ ,  $w_i = P(S_{0i})/P_0(S_{0i})$  are sampling weights, and  $Z_s = \sum w_i$  (see for example [17]). In our case,  $P$  is the true probability density  $e^{W^{(0)}}/Z$  and  $P_0$  is the probability density of the sample  $S_{0i}$  produced by the algorithm we describe, whose pdf  $P_0$  differs from  $P$  because the marginals used are only approximate.

The probability  $P_0$  of a sample  $S_0 = (s_{1,j}, \dots, s_{N,N})$  has to be computed as the sample is produced: the probability of each state of the spins in  $L_n$  is known and therefore the probability of the starting sample of  $L_n$  is known; each time one samples a spin in  $L_j$  for  $j < n$ , one has choices whose probabilities can be computed. As a practical matter, one must keep track not of the probabilities themselves but rather of their logarithms, or else one is undone by numerical underflow. Note that in the evaluation of  $P/P_0$  the factor  $Z^{-1}$  remains unknown, but as  $Z$  is common to all the samples, this does not matter. (And this remark can be made into an effective algorithm for evaluating  $Z$  and hence the entropy.) In practice I found it convenient to pick a value for  $Z$  so that  $E[\log(P/P_0)] = 0$ .

In practice, for lattices that are not very small, there is a significant range of weights, and there is a danger that the averaging will be dominated by a few large weights, which increase the statistical error. This issue has been discussed before (see for example [17]) where it is suggested that one resorts to ‘‘layering’’; this is indeed what we shall do, but more cautiously than suggested in previous work. Suppose one caps all weights at some value  $W$ , that is, replace the weights  $w_i$

by  $w'_i = \min(w_i, W)$ . The effective number of samples in the evaluation of the variance is  $N_W + \sum (w_i/w)$ , where  $N_W$  is the number of samples with  $w_i \geq W$ , and the summation is over the samples with  $w_i < W$ . Define the fraction  $f$  as the fraction of the samples such that  $w_i > W$  (so that  $w'_i = W$ ); as  $W$  increases the fraction  $f$  tends to zero. The averages computed by the algorithm here depend on  $f$  (or  $W$ ) and so does the statistical error; one has to ascertain that any result one claims is independent of  $f$ . Typically, as the size of the lattice increases, the range of weights increases, and therefore the effective number of samples decreases for a given number of samples  $N_s$ . What one has to do is check that the results converge to a limit as  $f$  decreases while the number of samples is still large enough for the results to be statistically significant. This may require an increase in  $N_s$  as  $N$  increases.

### 5. Bootstrapping the sampling

So far it has been assumed that one can sample the density  $e^{W^{(0)}}/Z$  well enough to compute the coefficients in the Kadanoff expansion (2-3) of the marginals. However, these coefficients are needed to make the sampling efficient when it would not otherwise be so, and the sampling has to be “bootstrapped” by iteration so it can be used to determine its own coefficients.

First, make a guess about the coefficients in (2-3), say, set

$$a_{i,j}^{\ell,m} = a_{i,j}^{\ell,m,0}$$

for the  $\ell$ -th coefficient at the point  $(i, j)$  in the sublattice  $L_m$ , where the numbers  $a_{i,j}^{\ell,m,0}$  are some plausible guesses. My experience is that it does not much matter what these guesses are; I typically picked them to be some moderate constants independent of  $i, j, m, \ell$ . Use these coefficients in a sampling procedure to find new coefficients  $a_{i,j}^{\ell,m,1}$ , and repeat as necessary. An iteration of this kind was discussed in [8], where it was shown that as the number of samples increases the error in the evaluation can be surprisingly small and that the optimal number of polynomials to use for a given overall accuracy depends on the number of samples. In the present work I found by numerical experiment that convergence is faster if, after one evaluates a new coefficient  $a_{i,j}^{\ell,m,r+1}$ , one sets in the next round

$$a_{i,j}^{\ell,m,r+1} = \frac{1}{2}(a_{i,j}^{\ell,m,r} + a_{i,j}^{\ell,m,r+1}).$$

I found experimentally that there is no advantage in computing these coefficients very accurately, indeed a relatively small number of samples is sufficient for each iteration, and two iterations have been sufficient for all the runs below.

### 6. Example 1: The two-dimensional Ising model

To check the algorithm and gauge its performance, we begin by applying it to the two-dimensional Ising model. I did not write a special program for this case and did not take advantage of the simplifications which arise when the coupling constants in the Hamiltonians are independent of location and one could replace four basis functions by the single function consisting of their sum, and the single expansion coefficient is the same at all points so that the projection can be averaged in space as well as over samples. Once expansion coefficients have been determined, they can be used to generate as many samples as one wants.

First, I computed the mean magnetization  $E[\mu]$ , where  $\mu = \frac{1}{N^2} \sum s_{i,j}$ ,  $1 \leq i, j \leq N$ , as a function of the temperature  $T$ . To calculate such means near  $T = T_c$  one needs a way to break the symmetry of the problem; this is usually done by adding a small asymmetric term  $\epsilon \sum s_{i,j}$  to the Hamiltonian, for example with  $\epsilon = \epsilon_0/N$ ,  $\epsilon_0 \sim 0.2$ . Adding such a field here works for small  $N$ , but as  $N$  increases, a value of  $\epsilon_0$  small enough not to disturb the final result may not suffice to bias the smallest lattice  $L_n$  in one direction. The remedy is to assign positive weights only to those spin configurations in  $L_n$  (where weights are explicitly known) such that  $\sum_{L_n} s_{i,j} \geq 0$ .

It may be tempting to introduce a symmetry breaker into the initial Hamiltonian  $W^{(0)}$ , add terms odd in the  $s_{i,j}$  to the series of linkages, and attempt to compute appropriate symmetry-breaking terms for the smaller lattices by a construction like the one above. This is not a good idea. The longer series is expensive to use and the computation of higher Hamiltonians is unstable to asymmetric perturbations, generating unnecessary errors.

In Table 1 we present numerical results for  $T = 2.2$  and different values of  $N$  compared with values obtained by Metropolis sampling with many sweeps of the lattice.  $N_s = 1000$  samples were used in each of two iterations to calculate the approximate marginals; once these are found one can inexpensively generate as many samples of the spins as wanted; here 1000 were used. Table 1 exhibits the dependence of the computed  $E[\mu]$  on the fraction  $f$  of weights which have been capped; the statistical error in the estimates of  $E[\mu]$  grows as  $f$  decreases, but more slowly than one would expect. For  $N = 16, 32, 64$  the results converge as  $f \rightarrow 0$  before the statistical error becomes large, but not when  $N = 128$ , and one should conclude that this value of  $N$  is too large for the present algorithm with so small a basis in the computation of marginals and so few samples. Even with  $N = 128$  one obtains a reasonable average ( $E[\mu] = .80$ ) if one is willing to use enough samples. Note also that the weights become large, and the calculations must be performed in double precision.

size of array	no. of samples $N_s$	$\log W$	$f$	$E[\mu]$	Metropolis
$16 \times 16$	1000	2	0.33	$0.74 \pm 0.01$	$0.81 \pm 0.01$
		4	0.08	$0.80 \pm 0.01$	
		6	0.00	$0.80 \pm 0.01$	
$32 \times 32$	1000	5	0.17	$0.76 \pm 0.01$	$0.81 \pm 0.01$
		7	0.10	$0.80 \pm 0.01$	
		9	0.04	$0.81 \pm 0.015$	
$64 \times 64$	1000	15	0.134	$.74 \pm .01$	$0.801 \pm 0.001$
		20	0.042	$0.77 \pm 0.01$	
		25	0.009	$0.80 \pm 0.01$	
		30	0.001	$0.80 \pm 0.015$	
$128 \times 128$	1000	25	0.074	$0.67 \pm 0.01$	$0.798 \pm 0.001$
		35	0.023	$0.70 \pm 0.01$	
		45	0.002	$0.74 \pm 0.02$	
		50	0.001	$0.75 \pm 0.05$	
				no convergence	

**Table 1.** Ising magnetization at  $T = 2.2$ .

We now turn to the determination of the critical temperature  $T_c$ . This can be obtained from the intersection of the graphs of  $E[\mu]$  versus  $T$  for various values of  $N$  (see for example [17; 16]); it is more instructive here to apply the construction in [9], based on the fact that if one expands the “renormalized” Hamiltonians in successive linkages, that is, if one finds the functions  $W^{(i)}$  such that the marginals on  $L_i$  are  $e^{W^{(i)}}/Z$ , using the series (2-3), then the sums of the coefficients in the series increase when  $T < T_c$  and decrease when  $T > T_c$ . For this construction to work, one needs enough polynomials for convergence, that is, so that the addition of more polynomials leaves the calculation unchanged. In the present case, this is achieved with 7 polynomials:  $\psi_1, \psi_2, \psi_3, \psi_4 = \sum s_{i,j} s_{i\pm 1, j\pm 1}$  (as above),  $\psi_5 = \sum s_{i,j} (s_{i+2,j} + s_{i,j+2} + s_{i-2,j} + s_{i,j-2})$ ,  $\psi_6 = \frac{1}{10} \sum s_{i,j} \sigma_{i,j}^3$ ,  $\psi_7 = \frac{1}{100} \sum s_{i,j} \sigma_{i,j}^5$ , where  $\sigma_{i,j} = s_{i+1,j} + s_{i,j+1} + s_{i,j-1} + s_{i-1,j}$ . The use of polynomials with higher powers of the  $s_{i,j}$  is essential (see for example [4]), and it is the more surprising that the approximate marginals calculated without them are already able to produce usable samples. The constant divisors in  $\psi_6, \psi_7$  are there to keep all the coefficients within the same order of magnitude. No advantage is taken here of the symmetries of the Ising model. In Table 2 I present the sums of the coefficients in the expansion as a function of the temperature  $T$  for the levels  $i = 2, 4, 6$  (where the lattices are mutually similar) in a  $N^2$  lattice with  $N = 16$  ( $N$  is chosen small for reference in the next section). From Table 2 one can readily deduce that  $2.25 < T_c < 2.33$ ; for

$T$	$i = 2$	$i = 4$	$i = 6$
2.20	1.63	2.16	2.71
2.25	1.50	1.77	1.88
2.26	1.49	1.73	1.50
2.28	1.45	1.65	1.40
2.30	1.41	1.50	1.30
2.32	1.36	1.40	1.13
2.33	1.35	1.34	1.15
2.35	1.30	1.27	0.95

**Table 2.** Sums of coefficients of Kadanoff expansion as a function of  $T$  for Ising model.

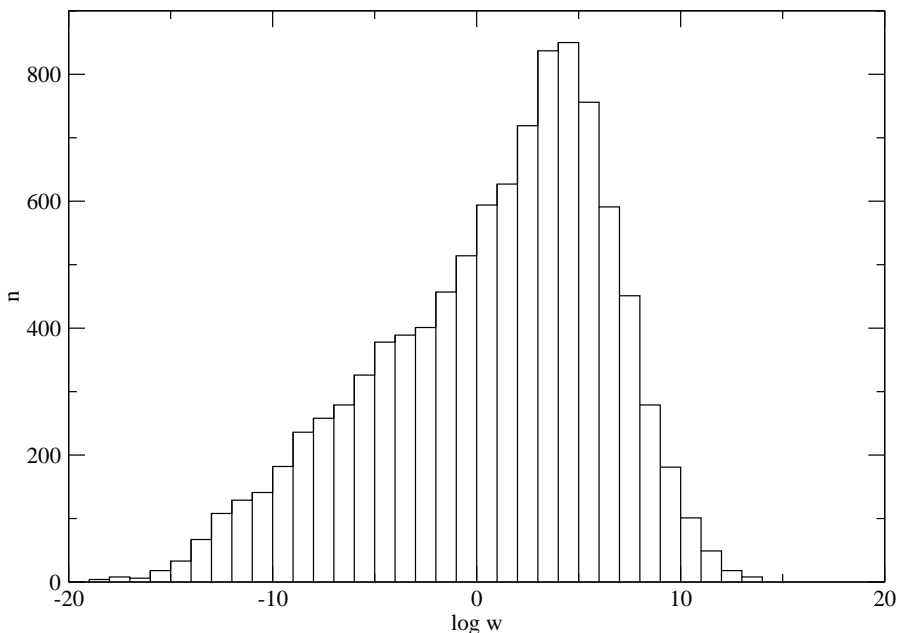
the value of  $T$  between these two bounds the sum of the coefficients oscillates as  $i$  increases. Taking the average of the two bounds (which are not optimal) yields  $T_c \equiv 2.29$  (the exact value is  $T_c = 2.269\dots$ ). A more careful analysis improves the result and so does a larger value of  $N$ . All the coefficients have the same sign, except occasionally when a coefficient has a very small absolute value.

For the sake of completeness I plotted in Figure 1 a histogram of the logarithms of the weights  $w_i$  for the Ising model with  $N = 32$  and  $10^4$  samples; the zero of  $\log w$  is chosen as described above. The cost per sample of an optimized version of this program for  $N = 32, 64$  is competitive with the cost of a cluster algorithm [22] and is significantly lower than that of a standard Metropolis sampler. It is not claimed that for the Ising model the chainless sampler is competitive with a cluster algorithm: as  $N$  increases the complexity of the present algorithm grows because one has to add polynomials and/or put up with a decrease in the number of effective samples, and one also has to do work to examine the convergence as  $f \rightarrow 0$ . The present sampler is meant to be useful when MCMC is slow, as in the next section.

## 7. Example 2: The Edwards–Anderson spin glass in three dimensions

We now use the chainless construction to calculate some properties of the EA spin glass [1; 5; 13; 16; 18; 24], and in particular, estimate the critical temperature  $T_c$ . The three-dimensional Edwards–Anderson spin glass model is defined by (2-1), where  $J_{i,j,k,\ell} = \beta \xi_{i,j,k,\ell}$ ,  $\xi_{i,j,k,\ell}$  are independent Gaussian random variables with mean zero and variance one, and  $\beta = 1/T$  is the inverse temperature. Periodic boundary conditions are imposed on the edge of the  $N^3$  lattice.

Let the symbol  $\langle \cdot \rangle$  denote a thermal average for a given sample of the  $J$ s, and let  $[\cdot]_{Av}$  denote an average over the realizations of the  $J$ s. Given two independent thermal samples of the spins  $S_{1,2} = \{s_{i,j,k}^{1,2}\}$ , we define their overlap to be  $q = N^{-3} \sum s_{i,j,k}^1 s_{i,j,k}^2$ , where the summation is over all sites in the lattice. The



**Figure 1.** Histogram of weights for the Ising model,  $N = 32$ ,  $10^4$  samples.

Binder cumulant [2; 16] is

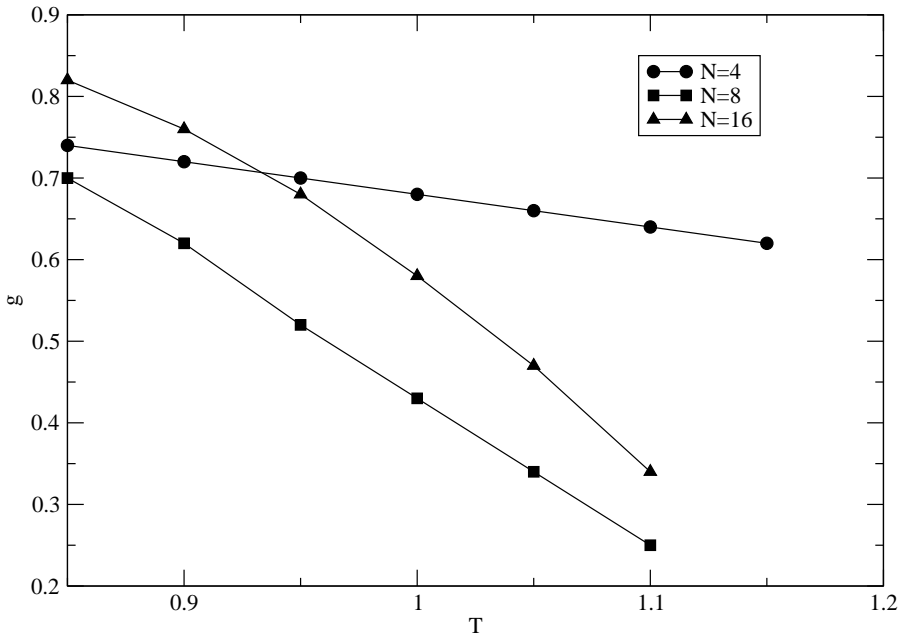
$$g = 0.5 \left( 3 - \frac{[\langle q^4 \rangle_T]_{Av}}{[\langle q^2 \rangle_T]_{Av}^2} \right).$$

The function  $g = g(T)$  is universal, and the graphs of  $g$  as a function of  $T$  for various values of the lattice size  $N$  should intersect at  $T = T_c$ .

The method presented above is applied to this problem. The only additional comment needed is that at every point of the lattice one has to invert a matrix generated by a random process, and occasionally one of these matrices will be singular or nearly so, and will produce unreliable coefficients, particularly for small samples sizes and low temperatures. As long as there are few such cases, there is no harm in jettisoning the resulting coefficients and replacing them by zeroes.

In Figure 2 I display the results obtained for this problem. The numerical parameters are: 2000 realizations of the  $J$ s, for each one of them 1000 samples for estimating the expansion coefficients and then 5000 samples for evaluating  $q$  and its moments. I used the bound  $\log W = 30$ , which produces a fraction of modified weights  $f = 0$  for  $N = 4$ ,  $f = 0.015$  for  $N = 8$  and  $f = .05$  for  $N = 16$ . The statistical error was hard to gauge; one can readily estimate the standard deviations of the numerical estimates of

$$[\langle q^4 \rangle_T]_{Av} \quad \text{and} \quad [\langle q^2 \rangle_T]_{Av}$$



**Figure 2.** The Binder cumulant  $g$  as a function of the temperature  $T$  in the three-dimensional AE model.

but these estimates are correlated and one therefore cannot use their separate standard deviations to estimate that of  $g$ . I simply made several runs for some of these computations and used the scatter of the results to estimate the statistical error. I concluded that the statistical error is around 1% for  $N = 4$  and 2–3% for  $N = 8, 16$ .

These three graphs taken separately approximate well the ones in the detailed computations of [16]. The graphs for  $N = 4$  and  $N = 16$  intersect at  $T = .93$ , which is the value of  $T_c$  deduced from the Binder cumulant computation in [16] (and which differs from the value  $T_c = .95$  deduced in the same paper from other considerations and which is likely to be right from the accumulated previous wisdom, as reported in that paper). The graph for  $N = 8$  is a little off from what one may expect, but again previous calculations, for example [16, Figure 7], also display comparable symptoms of unexpected waywardness. If one compares Figure 2 with [16, Figure 4], one sees other small discrepancies; for example, the values of  $g$  I obtained, in particular for  $N = 4$ , are smaller than those in [16] by a small but statistically significant amount; this cannot be the effect of “layering” (that is, the use of a bound  $W$ ) because for  $N = 4$  layering plays no role; it is hard to see how it can be produced by statistical error in either paper because the sample sizes are large enough. These small discrepancies are comparable to the ones observed in the best earlier computations. I have no explanation, except the general orneriness of



$T$	$i = 2$	$i = 5$	$i = 8$
0.6	3.07	3.95	3.73
0.9	2.70	3.90	3.42
1.0	2.43	3.34	2.76
2.0	6.20	8.51	8.87

**Table 3.** Sums of absolute values of Kadanoff coefficients for EA spin glass model.

the EA spin glass, as illustrated by the widely varying results for various exponents and thresholds summarized in [16]. These vagaries do not alter the fact that the algorithm of the present paper produces worthy results in a very difficult problem. A more detailed exploration of spin glasses will be published separately.

It is of interest in the present context to see how the coefficients in the Kadanoff expansion, used in the previous section to estimate  $T_c$  for the Ising model, behave in the three-dimensional spin glass. Now one needs more polynomials (20; the three-dimensional analogs of the ones in the preceding section plus others following the same pattern). The sums of all the coefficients add up to small numbers statistically indistinguishable from zero, as one may expect, so I display on Table 3 the sums of the absolute values of these coefficients for  $N = 16$  on self-similar lattices, which in the Ising case are equally able to exhibit  $T_c$  for this value of  $N$ . No bifurcation between growing and decreasing sums can be detected near  $T_c$ , illustrating differences between the phase transitions in the Ising and spin glass cases. Note the results for  $T = 0.6$ , a temperature hard to reach by a MCMC process.

The real question here is the efficiency and speed of the algorithm. What are needed are timing comparisons between an optimized version of it and optimized version of alternatives, such as the parallel tempering construction of [16]. This is not available. The least one can say is that the chainless sampler is highly competitive with others. Most of the computations in this paper (all but the ones for  $g$  at  $N = 16$ ) were first run on a single serial desktop machine.

## 8. Conclusions

A Monte Carlo sampling technique that relies on a fast marginalization rather than a Markov chain has been introduced, tested, and applied to a challenging test problem. The results demonstrate that it is a good alternative, especially for problems where the free energy has many minima and MCMC algorithms may be slow. Various improvements to this construction readily suggest themselves, based on more polynomials, better polynomials, and renormalization schemes other than

decimation. Related ideas, such as the parallel marginalization scheme proposed in [25], are also worth further investigation in the context of spin problems.

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