Exact sampling of corrugated surfaces

Sergio Caracciolo, Enrico Rinaldi and Andrea Sportiello

Dip. Fisica, Università degli Studi di Milano, and INFN, via G. Celoria 16, I-20133 Milano, Italy
E-mail: sergio.caracciolo@mi.infn.it, enrico.rinaldi@studenti.unimi.it and andrea.sportiello@mi.infn.it

Received 15 October 2008
Accepted 8 January 2009
Published 19 February 2009

Online at stacks.iop.org/JSTAT/2009/P02049
doi:10.1088/1742-5468/2009/02/P02049

Abstract. We discuss an algorithm for the exact sampling of vectors $\vec{v} \in [0,1]^N$ satisfying a set of pairwise difference inequalities. Applications include the exact sampling of skew Young Tableaux, of configurations in the Bead Model, and of corrugated surfaces on a graph, that is random landscapes in which at each vertex corresponds a local maximum or minimum. As an example, we numerically evaluate with high precision the number of corrugated surfaces on the square lattice. After an extrapolation to the thermodynamic limit, controlled by an exact formula, we put into evidence a discrepancy with previous numerical results.

Keywords: analysis of algorithms

ArXiv ePrint: 0810.2660
1. Introduction

Consider the following problem: given a grid $L \times L$, in how many ways can we fill the boxes with the numbers from 1 to $L^2$ in such a way that odd/even boxes are local maxima/minima? A typical allowed configuration for $L = 5$ is

\[
\begin{array}{cccccc}
6 & 20 & 10 & 18 & 16 \\
21 & 8 & 14 & 3 & 24 \\
9 & 15 & 11 & 12 & 7 \\
23 & 5 & 13 & 4 & 22 \\
2 & 17 & 1 & 25 & 19 \\
\end{array}
\]

A combinatorial more general setting is the following. Consider a direct acyclic graph $G = (V, \vec{E})$, with $N$ vertices: how many one-to-one maps $\sigma : V(G) \rightarrow \{1, \ldots, N\}$ exist such that, for each oriented edge $(ij) \in \vec{E}(G)$, $\sigma(i) > \sigma(j)$? The case of the square grid pertinent to corrugated surfaces corresponds to the graph

This wider framework includes, among other things, the counting of standard Young tableaux and standard skew Young tableaux [1, 2], as in the example below with the skew tableau $(6, 4, 4, 3) \setminus (3, 2)$:

\[
\begin{array}{cccc}
\text{\textcolor{gray}{gray}} & & \text{3} & \text{5} & \text{8} \\
\text{\textcolor{gray}{gray}} & \text{1} & \text{4} \\
2 & 6 & 10 & 12 \\
7 & 9 & \text{11} \\
\end{array}
\]

doi:10.1088/1742-5468/2009/02/P02049
Of course, given any ordering of the vertices in \( V(G) \), maps \( \sigma \) are naturally identified with permutations in \( \mathcal{S}_N \), and the fraction of maps satisfying all the constraints is given by

\[
Z_G = \frac{1}{N!} \# \{ \sigma \in S_N : \forall (ij) \in \vec{E}, \sigma(i) > \sigma(j) \}. \tag{1}
\]

There are many other applications in combinatorics and statistical mechanics. A connection is with the counting of acyclic orientations of a graph, a special evaluation of its Tutte polynomial, which is a \#P-hard problem (see, e.g., [3]).

For a given (unoriented) graph \( G = (V, E) \), an acyclic orientation \( \phi \) is a choice of orientation for the edges, such that no oriented cycles are created. Call \( A(G) \) the set of such \( \phi \)’s and, for any \( \phi \), call \( G(\phi) \) the corresponding oriented acyclic graph. Any one-to-one function \( \tau \) from \( V \) to a totally ordered set induces an acyclic orientation: just orient the edge \( (ij) \) from \( i \) to \( j \) if \( \tau(i) > \tau(j) \). Call \( G[\tau] \) the induced oriented acyclic graph. Given any ordering of the vertices, permutations are special cases of valid functions \( \tau \).

The uniform measure over \( \mathcal{S}_N \) easily allows exact sampling. However, it induces a biased measure over \( A(G) \) (through the natural function \( \phi(\tau) \) as the orientation \( \phi \) such that \( G[\tau] \equiv G(\phi) \)). The corresponding bias factor is exactly \( Z_{G[\tau]}^{-1} \), so that, for example,

\[
\frac{1}{N!} \sum_{\tau \in \mathcal{S}_N} Z^k_{G[\tau]} = \sum_{\phi \in A(G)} Z^{k+1}_{G(\phi)}, \tag{2}
\]

and in particular the average of \( Z_{G[\tau]}^{-1} \) is related to the cardinality of \( A(G) \).

Label the vertices with indices from 1 to \( N \). An equivalent formulation of the problem is to ask for the Lebesgue measure, in the interval \([0,1]^N\), of the vectors \( x = \{x_i\}_{1 \leq i \leq N} \) such that \( x_i \geq x_j \) for each oriented edge \( (ij) \) in the graph, oriented from \( i \) to \( j \). Indeed, at the aims of the \( N \)-dimensional measure, we can neglect configurations with repeated entries, and the constraint only depends on the ordering of the variables, so that

\[
Z_G = \int_{[0,1]^N} dx_1 \cdots dx_N \prod_{(ij) \in \vec{E}(G)} \theta(x_i - x_j) \tag{3}
\]

(here \( \theta(x) = 1 \) if \( x \geq 0 \) and \( \theta(x) = 0 \) if \( x < 0 \)). This alternative perspective gives justice to the name of ‘corrugated surfaces’ for the configurations on the grid (see figure 1) and makes explicit another specialization of the generalized model, the ‘bead model’ [4], corresponding to a realization on a square lattice rotated by an angle \( \pi/4 \), and the edges being directed, say, in the down-right and down-left directions.

The more general problem of understanding the statistics of local minima in a random landscape defined on a graph, which arises in the study of a point particle in a random potential or, for example, by looking at the energy landscape corresponding to configurations in many-body systems, was addressed in [5–7]. In particular in [7], instead of looking at typical configurations, the interest is shifted to the probability of large deviations, that is of configurations which are far from typical, as the configurations in which the local minima are maximally packed, i.e. corrugated surfaces. They provide both analytical (for Cayley trees) as well as numerical estimates (for hypercubic lattices) for the constant \( \gamma \) which controls the number of those configurations in the limit of large \( N \), as \( Z_G \sim \gamma^{-N} \). But the numerical results do not rely on Monte Carlo simulations.

doi:10.1088/1742-5468/2009/02/P02049
In this paper we present a Monte Carlo algorithm to ‘exactly’, that is without any bias, sample configurations $x \in [0, 1]^N$ satisfying our constraints, for an arbitrary given oriented acyclic graph $G$.

The algorithm runs under the paradigm of Propp and Wilson ‘coupling from the past’ (CFTP) [8], in a variant which allows for continuous-valued variables (the original CFTP setting is described for a discrete configuration space). As an application, we calculate numerically the large-size asymptotics (for $N \to \infty$) of the number of corrugated surfaces in two dimensions, with four digits of precision, under some hypothesis on the scaling exponents of the finite-size corrections (that we motivate theoretically in the following).

In light of this observation, it is not surprising that corrugated surfaces and the bead model allow for exact sampling using CFTP, as the relative discretized variants, hard-core lattice gas on the square lattice and lozenge tilings, are among the most studied applications of discrete CFTP or similar techniques (see [9] for the hard-core gas, plus [10] for a discrete-variable continuous-space version and [11] for lozenge tilings).

The extension of the method to continuous variables is not a big deal, and we do not claim much originality in this. However it is not either obvious a priori, as a crucial point is the possibility that two coupled random Markov chains reach coalescence, an event that could naively be thought to have zero probability in the Lebesgue sense. Some of these aspects have been already considered in the literature [12,13], while issues of a different sort, and more specific to our problem, are discussed in detail in the following.

2. Coupling from the past

As we said in the introduction, we used an ‘exact sampling’ algorithm, i.e. an algorithm that allows us to extract, in a finite time, a configuration in an ensemble with a given measure, without any bias. For a general discussion on Monte Carlo methods in statistical mechanics we refer to [14] where both the initialization bias, that is the source of systematic error related to ‘thermalization’, which is controlled by the exponential autocorrelation time, and the statistical error, controlled by the integrated autocorrelation time at

doi:10.1088/1742-5468/2009/02/P02049
 Exact sampling of corrugated surfaces

‘equilibrium’, are fully discussed. See also [15] for an example of rigorous bounds on the autocorrelation times related to physical observables for Metropolis algorithms.

The coupling from the past method (CFTP) also makes use of Markov chain processes. However, the two fundamental concepts of evolving a set of coupled chains, and analysing the dynamics backward in time, allow us to use a paradigm which leads to perfectly unbiased samples [8].

A coupled Markov chain is a process involving a set of configurations (say, \( k \) of them), which evolve under a dynamics being a valid dynamics for each chain, but using the very same sequence of randomly generated numbers in the different copies. This makes it a non-ergodic dynamics for the \( k \)-uple as a whole. In particular, if any two configurations become the same at some time \( t \), they will not anymore evolve into distinct configurations. The first time at which all \( k \) chains reach the same configuration is called the coalescence time and the coupled chain is said to have coalesced in this case.

Consider a conceptual experiment in which we follow the evolution of all the allowed configurations, with the chains weighted according to the measure on the ensemble. We have that, at least at the initial time, averages on the \( k \) copies of the chain correspond to statistical averages in the ensemble. Furthermore, this property must be preserved by the time evolution, and in particular must be true also in a limit \( t \to \infty \), in which, if the average time of coalescence is finite, we have a single configuration.

In order not to introduce a bias due to the ‘observation’ that the chains have coalesced, one must use a protocol of ‘looking backward’ in time, i.e. imagine performing the coupled-chain experiment above starting at a sequence of negative times, for example \( t_g = -2^g \), and stopping the dynamics at \( t = 0 \). Each finite state of the coupled chain has the property that averaging on all the surviving different copies, with the measure induced by the (averaged) time evolution, would provide the appropriate statistical averages, and in particular, at the first generation \( g \) such that the chain has coalesced, the only surviving final state is exactly sampled.

Following the full set of possible states is clearly infeasible. However, there is a case in which one can certify that all the states in the conceptual experiment above have coalesced, by just following a coupled Markov chain with \( k \) of order 1. This happens if the space of configurations is a poset, i.e. there is a structure of partial ordering \( \preceq \), and if there exist two special states \( O \) and \( I \) such that, for each \( X \) in the poset, \( O \preceq X \preceq I \) [16]. These conditions are satisfied in particular if the configuration space is a (mathematical) lattice. Furthermore, it is required that the (ergodic reversible) Markov chain dynamics, whose equilibrium distribution is the desired measure on the ensemble, preserves the ordering, i.e. the coupled evolution of two ordered configurations \( X_t \preceq Y_t \) leads to ordered configurations \( X_{t+1} \preceq Y_{t+1} \).

In this case, it suffices to work with \( k = 2 \), and initial states \( O \) and \( I \), in order to have that, if \( O \) and \( I \) have coalesced, all configurations in between also did it.

In summary, we can extract a general ‘CFTP protocol’ for sampling on a lattice. Given an ensemble, suppose that you can find a lattice structure on the space of configurations, and an ergodic reversible dynamics which preserves the ordering. Then, iteratively for \( g = 0, 1, 2, \ldots \), run the \( k = 2 \) coupled Markov chain with initial states \((O, I)\). It is important that, in the last \( 2^g \) times of the simulation at generation \( g + 1 \) you use the same set of random numbers used in all the \( 2^g \) times of the run at generation \( g \). Stop

doi:10.1088/1742-5468/2009/02/P02049
the simulation at the first generation $g_*$ such that the chain has reached coalescence: the exactly sampled configuration is the state at time $2^{g_*}$.

3. A CFTP algorithm for our model

Given our directed acyclic graph $G = (V, \overrightarrow{E})$, for each vertex $i$ we define $\mathcal{N}_+(i)$ as the set of vertices $j$ such that $(ji) \in \overrightarrow{E}(G)$, and $\mathcal{N}_-(i)$ as the set of vertices $j$ such that $(ij) \in \overrightarrow{E}(G)$. Then, a restatement of the constraint $\prod_{(ij)} \theta(x_i - x_j)$ is that, for each vertex $i \in V(G)$,

$$\max_{j \in \mathcal{N}_-(i)} (x_j) \leq x_i \leq \min_{j \in \mathcal{N}_+(i)} (x_j).$$

It is easy to devise an ergodic Monte Carlo chain with single-variable heat-bath moves. More explicitly, at each time step

(1) Choose $i$ at random uniformly in $V(G)$;
(2) Choose $z$ at random uniformly in $[0, 1]$;
(3) Replace $x_i$ by $z$ if it happens that

$$\max_{j \in \mathcal{N}_-(i)} (x_j) \leq z \leq \min_{j \in \mathcal{N}_+(i)} (x_j).$$

Note that, in the discrete formulation, such a dynamic would have been ‘quenched’ by the further, highly non-local constraint that all $\sigma(i)$’s are distinct.

The simple Monte Carlo chain above has the remarkable property of being suitable for CFTP, in the way described in section 2, this being another advantage of the continuous formulation, w.r.t. the one in terms of permutations. Consider the space $S \subseteq [0, 1]^N$ of valid vectors $x$, under the natural partial ordering $x \preceq y$ if $x_i \leq y_i$ for all $i \in V(G)$. For any graph $G$, this space is a lattice, as there are both an $O$ and an $I$ element, corresponding to the vectors $\vec{0}$ and $\vec{1}$ respectively.

Then, the second condition for CFTP is that, given two configurations $x$ and $y$ at time $t$ such that $x \preceq y$, the coupled time evolution preserves the ordering. This is easily seen with the help of the crucial observation that, for any vertex $i$, with the definitions

$$j' = \arg\min_{\mathcal{N}_+(i)} (y_j); \quad j'' = \arg\max_{\mathcal{N}_-(i)} (x_j);$$

one has

$$\min_{j \in \mathcal{N}_+(i)} (x_j) \leq x_{j'} \leq y_{j'} = \min_{j \in \mathcal{N}_+(i)} (y_j);$$

$$\max_{j \in \mathcal{N}_-(i)} (x_j) = x_{j''} \leq y_{j''} \leq \max_{j \in \mathcal{N}_-(i)} (y_j).$$

Call

$$x_+ = \min_{j \in \mathcal{N}_+(i)} (x_j); \quad x_- = \max_{j \in \mathcal{N}_-(i)} (x_j).$$

The range of values in which the new candidate variable $z$ is accepted in $x_i$ is the interval $[x_-, x_+]$, and similarly for $y$. The statement in (6) is that $x_\pm \leq y_\pm$ if $x \preceq y$. If $x_+ \geq y_-$, there is a probability $(x_+ - y_-)/(y_+ - x_-)$ that, given that a move occurs, the number of indices $i$ for which $x_i \equiv y_i$ increases by one. If instead $x_i \equiv y_i$ at some time (and in

doi:10.1088/1742-5468/2009/02/P02049
this case it must be $x_+ \geq y_-$, there is a probability $1 - (x_+ - y_-)/(y_+ - x_-)$ that this number decreases by one. Calling $C(x, y) = \{i : x_i \equiv y_i\}$, we can define a distance parameter $d(x, y) = |C(x, y)|$, and the reasonings above describe a non-trivial hopping dynamics in the parameter $d(x, y) \in \{0, \ldots, N\}$. The chain starts from $d(x, y) = N$ and reaches coalescence when $d(x, y) = 0$, which is thus a fixed point of the induced restricted dynamics.

One could naively think that the extrema $d = 0$ and $N$ are strongly repulsive, in a way that becomes stronger with lattice size, because of ‘entropic reasons’ (e.g. for $d = 0$, if $|C| = \mathcal{O}(N)$ and $|V(G) \setminus C| = \mathcal{O}(1)$, we have a relative factor $1/N$ for choosing an index in the second set). At least in graphs with low degree, say bounded by $k$, this is the case for $d = N$, but not for $d$ near 0. Indeed, if the dynamics chooses a site in $C$ such that all its neighbours are in $C$, the distance cannot increase at that time step, so that the ratio between the two rates $d \to d \pm 1$ is bounded by $k$.

4. From exact sampling to the calculation of the free energy

It is well known [17] (see also section 3.2 of [18]) that the problems of (approximated) counting and of uniform sampling are closely related. In particular, there is a way of calculating numerically the free energy of a model of interest if we can generalize the model introducing an extra parameter $\epsilon$ such that

- at $\epsilon = 1$ we recover the model of interest;
- at $\epsilon = 0$ the free energy is known exactly;
- exact sampling is available in the range $\epsilon \in [0, 1]$;
- the (unnormalized) Gibbs measures $\mu_\epsilon$, for different values of $\epsilon$, are absolutely continuous (in either direction).

Actually, instead of the last point, it is sufficient to have the weaker but more technical statement of having a Radon–Nikodym derivative of a measure at a value $\epsilon$ w.r.t. a measure at a value $\epsilon'$, for a suitable set of pairs $(\epsilon, \epsilon')$ (see [19] for the pertinent definitions). Indeed, if, for example, for $\epsilon < \epsilon'$ we have $\mu_\epsilon \ll \mu_{\epsilon'}$, then we have a function $g_{\epsilon, \epsilon'}(x)$ such that

$$|\mu_\epsilon| := \int d\mu_\epsilon(x) = \int g_{\epsilon, \epsilon'}(x) d\mu_{\epsilon'}(x),$$  \hspace{1cm} (8)

and thus, by defining the free energy as $F(\epsilon) = \ln |\mu_\epsilon|$ (we neglect the constant factor $-1/\beta$ customary in thermodynamics), we have

$$F(\epsilon) = F(\epsilon') + \ln \langle g_{\epsilon, \epsilon'} \rangle_{\epsilon'},$$  \hspace{1cm} (9)

which can be used telescopically in order to obtain $F(1)$ from $F(0)$ and the evaluation of $\ln \langle g_{\epsilon_i, \epsilon_{i+1}} \rangle$ through the exact sampling algorithm run at some sequence of $\epsilon_i$s, sufficiently dense that the statistics of $g_{\epsilon_i, \epsilon_{i+1}}$ is significant. Also, if one can define

$$\tilde{g}(\epsilon) = \lim_{\delta \to 0} \frac{\ln \langle g_{\epsilon + \delta, \epsilon} \rangle_\epsilon}{\delta},$$  \hspace{1cm} (10)
and this function is smooth in $\epsilon$, the free energy for the model of interest would be given by

$$F(1) = F(0) + \int_0^1 d\epsilon \tilde{g}(\epsilon),$$

and it could be more efficient to find a reasonable continuous fit of $\tilde{g}(\epsilon)$ from simulations run at some sequence of $\epsilon$'s.

In our case of corrugated surfaces, for a configuration $x$ define $W[x] \subset V(G)$ as the set of vertices being maxima and in the range $[0, \frac{1}{2}]$, union the ones being minima and in the range $[\frac{1}{2}, 1]$. Call $m(x) = |W[x]|$. Then choose

$$\mu_{\epsilon}(x) = \epsilon^m(x) \prod_{(ij) \in E} \theta(x_i - x_j).$$

It is evident that $\epsilon = 1$ corresponds to our model and that at $\epsilon = 0$ we just have $Z_G = 2^{-N}$.

The Markov chain introduced in section 3 is easily generalized to the introduction of the parameter $\epsilon$. Just the second point, where we ask to extract $z$ uniformly in the interval $[0, 1]$, has to be replaced by the measure on $[0, 1]$:

$$p_{\epsilon}^{(\pm)}(z) = \frac{2}{1 + \epsilon} \left( \epsilon + (1 - \epsilon) \theta \left( \pm \left( z - \frac{1}{2} \right) \right) \right),$$

with $+/-$ if we are performing the move respectively on the position of a maximum or a minimum. The plot of $p_{\epsilon}^{(\pm)}(z)$ is just

Specialization of the quantity in (10) is easily achieved:

$$g_{\epsilon, \epsilon'}(x) = \left( \frac{\epsilon}{\epsilon'} \right)^m(x)$$

and, taking the limit,

$$\tilde{g}(\epsilon) = \frac{1}{\epsilon} \langle m(x) \rangle_{\epsilon}.$$

The apparent singularity at $\epsilon = 0$ is not there, as $\langle m(x) \rangle_{\epsilon}$ vanishes linearly with $\epsilon$. Also, the potential risk of having an explosion of data noise at $\epsilon = 0$ is easily avoided: as this point is the trivial limit of the theory, it is easy to match the data near $\epsilon = 0$ with the first few terms of a cluster expansion. Call $G(L)$ the graph corresponding to a grid of side $L$ and define the intensive free energy as

$$f(\epsilon; L) = \frac{1}{L^2} \ln Z_{G(L)};$$

then the cluster expansion, in powers of $\epsilon$ and inverse powers of $L$, gives

$$f(\epsilon; L) = -\ln 2 + \frac{\epsilon}{5} - \left( \frac{4\epsilon}{15} \right)^2 + \frac{\epsilon}{5L} + \mathcal{O} \left( \epsilon^3, \frac{\epsilon^2}{L}, \frac{\epsilon}{L^2} \right).$$
The observable $W[x]$ also has an appealing interpretation. It is clear that no adjacent vertices can be simultaneously in $W$ so, for each configuration $x$, $W$ is a hard-core gas configuration (or an independent set). The parameter $\epsilon$ plays the role of an effective fugacity in the gas and, although the correspondence is not perfect, we can imagine that, if any criticality at all appears in the model, it will be in the same universality class as the two-dimensional hard-core lattice gas.

For the general case, one can alternatively use the intuitive ‘temperature’ parametrization. Allow for all configurations $x \in [0, 1]^N$ and define $h(x)$ as the number of edges whose constraint is not satisfied. Then we can write

$$\mu_\epsilon(x) = \prod_{(ij) \in \bar{E}} (\epsilon \theta(x_i - x_j) + (1 - \epsilon)).$$

(17)

Again $\epsilon = 1$ corresponds to our model, while at $\epsilon = 0$ we just have $Z_G = 1$. Similarly

$$g_{\epsilon, \epsilon'}(x) = \left( \frac{1 - \epsilon}{1 - \epsilon'} \right)^{h(x)}$$

(18)

and, taking the limit,

$$\tilde{g}(\epsilon) = -\frac{1}{1 - \epsilon} \langle h(x) \rangle_\epsilon.$$

(19)

Again the apparent singularity at $\epsilon = 1$ is not there, as $\langle h(x) \rangle$ vanishes linearly at that point. However, in this case the increase of noise at $\epsilon = 1$ is unavoidable, this being the reason why we have chosen the ad hoc parametrization (12) for our numerical simulations of corrugated surfaces.

5. Numerical data for corrugated surfaces

In order to obtain a reliable estimate we performed our simulations for values of $L = 16, 32, \ldots, 256$ and at 20 different values of $\epsilon$, equally spaced, in the relevant interval, in the parametrization $\epsilon/(1 + \epsilon)$. For each value of $L$ and $\epsilon$, we performed $10^4$ independent runs, providing us a set of numerical values for the quantities

$$\frac{\partial}{\partial \epsilon} f(\epsilon; L) = \frac{\langle m(x) \rangle_\epsilon}{L^2 \epsilon}.$$ 

(20)

For each value of $\epsilon$ in our analysis, the distribution of $m(x)$ in the output configurations is well fitted by a Gaussian (cf. for example figure 2), in agreement with the fact that, if $m(x)$ is a good order parameter, as we expect from the analogy with the hard-core lattice gas, we are in a regime with a single Gibbs phase. We checked that our numerical implementation provides exactly the results on the non-trivial case $L = 3$ which can be computed analytically. For the larger values of $L$, at each value of $\epsilon$, the numerical values of $\partial/\partial \epsilon f(\epsilon; L)$ are in good agreement with a finite-size description in which the first correction scales with $1/L$. So, in a fit of the form

$$\frac{\partial}{\partial \epsilon} f(\epsilon; L) \sim \frac{\partial}{\partial \epsilon} f(\epsilon) + \frac{A(\epsilon)}{L} + \frac{B(\epsilon)}{L^2},$$

(21)
Figure 2. Distribution of $L^2 m(x)$, averaged over $10^4$ exactly sampled configurations, on a system with size $L = 256$, at $\epsilon = 1$. The fit is with a Gaussian.

Figure 3. Numerical data for the function in (22). The natural error bars are invisible. In the figure, we magnified the errors by a factor of 100 in order to highlight the different relative errors in the two regimes of $\epsilon \to 0$ and $\epsilon = O(1)$. The linear behaviour at $\epsilon = 0$ is deduced from the cluster expansion in (16).

we extrapolated the asymptotic values

$$\frac{\partial}{\partial \epsilon} f(\epsilon) = \lim_{L \to \infty} \frac{\langle m(\epsilon) \rangle_{\epsilon}}{L^2 \epsilon}.$$  

(22)

A scrupulous statistical analysis of the errors, just within the (well-verified) assumption on the exponent of the leading finite-size correction, leads to the results in figure 3. Finally, numerical integration of a polynomial interpolation of the data (with a polynomial of degree 5, determined by analysis of structure in the errors) provided us
with the result
\[ f = -0.53967 \pm 0.00054. \] (23)

The parameter $\gamma$ is obtained from $\gamma = \exp(-f)$. Our numerical analysis on the square lattice gives
\[ \gamma = 1.7154 \pm 0.0009, \] (24)
with purely statistical errors. This must be compared with the previous numerical estimate [7]
\[ \gamma_{MM}(2) = 1.6577 \pm 0.0006, \] (25)
which is definitely outside the estimated errors. Even if the difference appears to be small it is interesting to observe that, as the estimate in [7] for the three-dimensional cubic lattice is
\[ \gamma_{MM}(3) = 1.7152 \pm 0.0010, \] (26)
the discrepancy is of the same size of the estimated difference between the two-and three-dimensional constants.

6. Analysis of the times to coalescence

According to the ‘ordinary’ CFTP protocol (not the Read-Once protocol of [10]), the running times for each size, and each independent instance is essentially a power of 2, say, $2^g$. This means that the average complexity of the algorithm is described through some probability for the $\text{generation}$ parameter $g$, at side $L$, that we call $p_L(g)$:
\[ \text{Time}(L) \sim \sum_g 2^g p_L(g). \] (27)

It is a tautology that this time is finite provided that $p_L(g)$ has a Laplace transform at the value $-\ln 2$. It comes out that, in our range $\epsilon \in [0,1]$, the times grow monotonically with $\epsilon$, and even at the hardest point $\epsilon = 1$ the histogram $p_L(g)$ takes its leading contribution from one or two values of $g$. At fixed $g$, the plot of $p_L(g)$ in the variable $L$ instead looks like a smooth bell-shaped curve in the range $[0,1]$ (cf. figure 4) and it is fairly safe to interpolate the (continuous) value $L(g)$ of $L$ at which the curve for $g$ and the one for $g+1$ do cross. Given this regular behaviour, the scaling of $L(g)$ with $g$ must be related to the scaling of the complexity, in particular, if $g(L)$ is the functional inverse of the (obviously monotone) $L(g)$, then
\[ \text{Time}(L) \sim 2^{g(L)}. \] (28)

The data are well fitted by a curve of the form
\[ g(L) \propto L^2 \ln L, \] (29)
so the complexity seems to be only logarithmically super-linear in the number of degrees of freedom.

As we discussed in section 4, the pictorial interpretation of the observable $W[x]$ suggests that our model of corrugated surfaces, in its continuation to arbitrary values of
Exact sampling of corrugated surfaces

Figure 4. On the left, plots of $p_L(g)$ in the variable $L$, for $g = 8, \ldots, 19$. On the right, table of the values $L(g)$ interpolated from the data. Errors are estimated to be on the last digit.

$\epsilon$, is in the same universality class as the hard-core lattice gas, so it was natural to expect that, analogously to what is proven for this model [20,21], the average coalescence time is $\sim n \ln n$ for Glauber dynamics at sufficiently small fugacities (in agreement with (29) above), while it becomes worst-case hard at sufficiently large fugacities, these values being lower and upper bounds to the ‘physical’ critical values $\epsilon^*$ (the gap being originated by technicalities in the proof procedure). It is not inconceivable that, for our system, all the range $\epsilon \leq 1$ has fast coalescence times.

Furthermore, fast convergence would imply a choice of parameters which are far from a critical point and correspond to a single thermodynamic phase [22,23], and this would imply in turns that finite-size corrections to intensive observables scale with the ratio perimeter/area, i.e. with $L^{-1}$ in our two-dimensional case. This justifies the treatment of the finite-size corrections that we have done in section 5.

7. Conclusions

We have pointed out how the method of coupling from the past may be fruitfully applied to problems with variables assuming values on a continuum domain, and how a one-variable heat-bath Monte Carlo chain is suitable for CFTP in an interesting problem in this class: the uniform sampling of height functions satisfying a set of inequalities described by an acyclic graph.

As a specific example, we performed a numerical simulation for the model of corrugated surfaces in order to determine the value of the free energy. Our precision goal was to have error bars much below the order of magnitude of the discrepancy between ours and the estimate, obtained without using a Monte Carlo method, that appears in Majumdar and Martin [7]. To this aim, the use of an exact sampling method in connection with an exact formula for the extrapolation to the thermodynamical limit has been useful in order to rule out any possible source of systematic errors.

We have achieved our goals with a relatively small numerical effort, because the model of corrugated surfaces appears to be a special value of a one-parameter family of...
models, in the universality class of the two-dimensional hard-core lattice gas, in the low-density phase. In this case, as expected from the literature, the mixing times are only logarithmically super-linear and the coalescence time for the coupled chain is of the same order of magnitude of the mixing time of the ordinary Markov chain. As a final comment, we advise that, in this regime, the strong control over the errors in the CFTP overwhelms the small gain in terms of computational times of other Monte Carlo algorithms.

Acknowledgments

We thank L Cantini and C Boutillier for fruitful discussions.

References

[1] Aitken A C, The monomial expansion of determinantal symmetric functions, 1943 Proc. R. Soc. Edinburgh A 61 300
[2] Stanley R P, On the enumeration of skew Young tableaux, 2003 Adv. Appl. Math. 30 283
[3] Laos B, Orientations Acycliques et le Polynôme Chromatique, 2001 Eur. J. Comb. 22 1101
[4] Boutillier C, The bead model and limit behaviors of dimer models, 2006 arXiv:math/0607162
[5] Hivert F, Nechaev S, Oshanin G and Vasilyev O, On the distribution of surface extrema in several one- and two-dimensional random landscapes, 2007 J Stat. Phys. 126 243 [arXiv:cond-mat/0509584]
[6] Oshanin G, Voituriez R, Nechaev S, Vasilyev O and Hivert F, Random patterns generated by random permutations of natural numbers, 2007 Eur. Phys. J. Special Topics 143 143 [arXiv:cond-mat/0609718]
[7] Majumdar S N and Martin O C, The statistics of the number of minima in a random energy landscape, 2006 Phys. Rev. E 74 061112 [arXiv:cond-mat/0609735]
[8] Propp J and Wilson D B, Exact sampling with coupled Markov chains and applications to statistical mechanics, 1996 Random Struct. Algorithms 9 223
[9] Fill J A and Huber M, The randomness recycler: a new technique for perfect sampling, 2000 41st Annual Symp. on Foundations of Computer Science p 503 [arXiv:math.PR/0009242]
[10] Wilson D B, How to Couple from the Past using a Read-Once source of randomness, 2000 Random Struct. Algorithms 16 85
[11] Wilson D B, Mixing times of lozenge tiling and card shuffling Markov chains, 2004 Ann. Appl. Probab. 14 274 [arXiv:math.PR/0102193]
[12] Murdoch D J and Green P J, Exact sampling from a continuous state space, 1998 Scand. J. Stat. 25 483
[13] Mitha F, Perfect sampling on continuous state spaces, 2003 PhD Thesis University of North Carolina at Chapel, Dept of Statistics
[14] Sokal A D, Monte Carlo methods in statistical mechanics: foundations and new algorithms, 1997 Functional Integration: Basics and Applications Proc. Cargèse Summer School (Sept. 1996) (Nato ASI Series B: Physics) vol 301, ed C De Witt-Morette, P Cartier and A Falacci (Dordrecht: Kluwer-Academic/Plenum)
[15] Caracciolo S, Pelissetto A and Sokal A D, A General limitation on Monte Carlo algorithms of metropolis type, 1994 Phys. Rev. Lett. 72 179 [arXiv:hep-lat/9307021]
[16] Birkhoff G, 1979 Lattice Theory 3rd edn, vol 25 (Washington, DC: American Mathematical Society Colloquium Publications) Amer. Math. Soc.
[17] Jerrum M, Valiant L G and Vazirani V V, Random generation of combinatorial structures from a uniform distribution, 1986 Theor. Comput. Sci. 43 109
[18] Jerrum M, 2003 Counting, Sampling and Integrating: Algorithms and Complexity (Lectures in Mathematics. ETH Zürich) (Basel: Birkhäuser)
[19] Ambrosio L, Gigli N and Savaré G, 2005 Gradient Flows in Metric Spaces and in the Space of Probability Measures (Lectures in Mathematics. ETH Zürich) (Basel: Birkhäuser)
[20] Luby M and Vigoda E, Fast convergence of the Glauber dynamics for sampling independent sets, 1999 Random Struct. Algorithms 15 229
[21] Dyer M and Greenhill C, On Markov chains for independent sets, 2000 J. Algorithms 35 17
[22] Weitz D, Combinatorial criteria for uniqueness of Gibbs measures, 2005 Random Struct. Algorithms 27 445
[23] Weitz D, Mixing in time and space for discrete spin systems, 2004 PhD Thesis UC Berkeley

doi:10.1088/1742-5468/2009/02/P02049