Inverse Monte Carlo Renormalization Group Transformations for Critical Phenomena

Dorit Ron
Department of Computer Science and Applied Mathematics, Weizmann Institute of Science, Rehovot 76100, Israel

Robert H. Swendsen
Physics Department, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213

Achi Brandt
Department of Computer Science and Applied Mathematics, Weizmann Institute of Science, Rehovot 76100, Israel
(Received 24 June 2002; published 18 December 2002)

We introduce a computationally stable *inverse* Monte Carlo renormalization group transformation method that provides a number of advantages for the calculation of critical properties. We are able to simulate the fixed point of a renormalization group for arbitrarily large lattices without critical slowing down. The log-log scaling plots obtained with this method show remarkable linearity, leading to accurate estimates for critical exponents. We illustrate this method with calculations in two- and three-dimensional Ising models for a variety of renormalization group transformations.

DOI: 10.1103/PhysRevLett.89.275701 PACS numbers: 64.60.Ak, 05.50.+q, 05.10.Cc, 05.10.Ln

The renormalization group (RG), which has become central to any discussion of critical phenomena, is generally regarded as not having an inverse, making it really a semigroup. There are serious reasons for avoiding an inverse transformation in many cases, as we discuss below. However, as we demonstrate in this Letter, there can be considerable advantages to turning the usual renormalization group analysis around to use an *inverse* renormalization group (IRG) transformation to generate large systems that correspond to the fixed point (FP) of a renormalization group. The striking advantage of this approach is that it is completely free of critical slowing down.

A kind of inverse RG transformation to generate configurations of the Ising model on a large lattice was carried out by Compagner, Hoogland, and Blöte in the late 1970s [1], but the first attempt to use an inverse renormalization group transformation for efficient simulations was made by Brandt and Ron [2]. They performed what they called "coarse-to-fine Monte Carlo acceleration" under the assumption that they knew the structure of the renormalized Hamiltonians at each stage. Although their method is completely valid in principle, it suffers from the fact that the Hamiltonians at each stage are not known and would have to be computed individually.

The basic algorithm used in this Letter is essentially the same as that introduced by Brandt and Ron [2]. However, instead of attempting to simulate the properties of a nearest-neighbor model, we develop approximations for the simulation of the fixed point of an RG transformation. The difference is crucial for the efficient calculation of critical properties.

A normal Monte Carlo renormalization group (MCRG) calculation begins with a Monte Carlo (MC) simulation performed on a relatively large system [3]. For each generated configuration, a renormalized configuration can also be generated by grouping the spins into blocks and assigning a single, renormalized spin to each block on the basis of some rule. For example, a "majority-rule" RG transformation for an Ising model would assign a block spin according to the sign of the majority of spins, with a random number being used in case of a tie.

By such transformations, the linear dimension of the lattice would be reduced by a factor of b, and the number of spins would be reduced by a factor of b^d, where d is the dimension of the system. If the original Hamiltonian was at a critical point, the repeated transformations would carry the renormalized Hamiltonians toward the fixed point. If not, each iteration would move away from the critical sheet. The trajectories flow toward the fixed point in all directions except one. For a normal MCRG calculation, every critical system has an RG trajectory that flows toward the FP.

The inverse RG transformation requires the knowledge of both the RG transformation and the Hamiltonian of the previous renormalization step [2]. Using the $d = 2$, 2×2 majority-rule Ising RG as an example, each spin is replaced by a 2×2 block of spins of the same sign, and an MC simulation is carried out with the constraint that configurations are restricted to those that are compatible with the smaller system. Proposed spin flips that would violate the compatibility condition are rejected. If a spin flip would result in a block with an equal number of positive and negative spins, the acceptance probability of the move is divided by two. Brandt and Ron called this step "compatible Monte Carlo" (CMC) for obvious reasons [2]. Because of the local nature of the relaxation, CMC has a very small, size-independent correlation time, even for systems at criticality. This gives a configuration

corresponding to a lower level of renormalization on a larger lattice. By iteration of this transformation, arbitrarily large lattices can be generated.

Each sequence of inversely renormalized lattices begins with a small lattice with a short relaxation time, which makes it easy to produce independent configurations. Since the larger lattices are all based on the smallest lattices, every produced configuration for any lattice size is independent.

Before discussing the approximations necessary for this calculation, first assume that we could carry out this procedure exactly. For the IRG, the deviation from the FP in the relevant direction would *decrease* by a factor of $1/\lambda_1$ (where $\lambda_1 > 1$ is the relevant eigenvalue of the RG transformation), moving the system onto the critical sheet. On the other hand, the deviations from the FP in all irrelevant directions would *increase* by factors of $1/\lambda_j > 1$, where $\{\lambda_j | j > 1\}$ is the set of irrelevant eigenvalues, since all irrelevant eigenvalues are less than 1. In fact, most of the irrelevant eigenvalues are very small, so that tiny deviations from the FP would be greatly magnified by this procedure.

Curiously enough, while this feature of the exact inverse transformation makes it unsuitable for application to general Hamiltonians, the approximate inverse transformations we apply to the fixed point Hamiltonian are stable and efficient.

The key feature to notice is that while the MC generation of a renormalized configuration requires only the original configuration and a well-defined RG, the inverse process requires not only the coarse configuration, but also the inversely renormalized Hamiltonian. It is the exact inversely renormalized Hamiltonian that develops the pathological expansion of the irrelevant operators.

In this Letter, we apply IRG transformations to the fixed point Hamiltonian of the transformation, which eliminates the pathology of inversely renormalized Hamiltonians. The approximations that we use also eliminate numerical instabilities that could arise from the divergence of irrelevant operators under the IRG. A final advantage of this approach is that it uses the *same* Hamiltonian at every level.

Although we cannot calculate the FP Hamiltonian exactly for any known RG transformation, several methods have been developed for approximating such Hamiltonians. Swendsen developed a method for calculating renormalized and fixed point Hamiltonians [4–6]. Brandt and Ron developed methods for calculating systematically better approximations for the FP Hamiltonian in terms of tables of conditional probabilities [2]. Blöte *et al.* developed an optimized RG transformation and found a good approximation for its FP Hamiltonian [7]. We have applied the results of all of these calculations to the creation of approximate realizations of the IRG. Gupta and Cordery also developed a method for calculating renormalized Hamiltonians [8], as did Ron and Swendsen [9]. However, since these methods have not been used to determine fixed point Hamiltonians, we have not included them.

As a first application of the IRG method to approximations for the fixed point Hamiltonian, we have used finite-size scaling of the large lattices available through these calculations to calculate the critical exponent ratio γ/ν and the value of η. The ratio γ/ν was obtained from a log-log plot of the magnetic susceptibility as a function of the linear system size, since the magnetic susceptibility χ is proportional to $L^{\gamma/\nu}$. The exponent η was obtained from the spin-spin correlation function, which decays as $r^{-(d-2+\eta)}$, using the finite-size scaling of the function at $r = L/4$. All simulations started on a 4×4 lattice, employing 20 CMC sweeps on increasingly larger grids with periodic boundary conditions throughout. The largest lattices used were 1024×1024, although the method is not limited to this size.

There are two types of errors involved in calculating γ/ν: One is due to the inaccurate fixed point Hamiltonian that we used; the other is due to the statistical and finite-size effects. It turned out that the finite-size errors in all our tests were much smaller than the statistical errors. We have calculated the latter by comparing runs with different amount of statistics. The number of independent configurations needed to obtain high accuracy is rather small: 10^5 configurations are sufficient to obtain small statistical errors of about 0.003%, provided the observables of all lattices are measured from the *same* simulation to guarantee the compatibility of all of them to each other. If, however, the observables are calculated separately from different runs for different lattice sizes, the statistical errors are at least 50 times larger.

The first approximate realization of the IRG that we have tried uses the nearest-neighbor, two-dimensional Ising model at its critical point as an approximation for the fixed point Hamiltonian of the 2×2 majority-rule RG. This is clearly a very poor approximation, since the FP Hamiltonian of this RG transformation is known to be quite far from the nearest-neighbor model. However, the results of this calculation, $\gamma/\nu = 1.761\,95(2)$, are surprisingly good. The error in the estimate of γ/ν compared to the known value of $\gamma/\nu = 1.75$ is only 0.7%.

A similar simulation was tried by Brandt and Ron in [2] for the purpose of accelerating calculations of observables for the nearest-neighbor Hamiltonian. The accuracy there was enhanced by adding a small number of regular (unconstrained) MC passes following the CMC sweeps. This step was called "postrelaxation." However, since postrelaxation disturbs the compatibility of the results of various levels, as we have confirmed by calculations, we have not included it in the present work.

To improve the approximation, we have used an approximated FP Hamiltonian given by a seven-coupling Hamiltonian as calculated by Swendsen [5], using comparisons of different methods for calculating

correlation functions. This approximation gives $\gamma/\nu = 1.749\,91(3)$, which represents a remarkably small error of only 0.005%.

We have performed several other calculations for the two-dimensional Ising model using the Brandt-Ron representation of renormalized Hamiltonians and their procedures for determining fixed point Hamiltonians. These calculations were also successful, but space does not permit us to explain the involved computations and give the results here. They will be presented in a separate publication [10].

For the three-dimensional model, we have neither the exact location of the critical point of the nearest-neighbor model nor exact values of the critical exponents to compare our results with. However, we do have numerical estimates of the locations of fixed points for a variety of RG transformations. This lets us consider a variety of ways to implement the IRG approach. In these simulations, we have started from a $4 \times 4 \times 4$ lattice. Larger lattices were obtained by employing 20 CMC sweeps up to a linear size of 128 using again periodic boundary conditions. Each computation generated only 5000 independent configurations.

As was the case for the two-dimensional model, we performed many more computations than we can report here, using transformations and fixed point Hamiltonians calculated by Blöte *et al.* [7] and Swendsen, as well as several calculations based on the Brandt-Ron representation. The simple nearest-neighbor, three-dimensional Ising model at its critical point gave an approximation of $\gamma/\nu = 1.9158(5)$ with a deviation of about 2.3% from the generally accepted value, i.e., $\gamma/\nu = 1.962(2)$ [7]. The deviation of this case is larger than for the two-dimensional case; however, it is still rather good for such an obviously bad approximation. To present a clear illustration of the method, we have then used an estimate of the FP Hamiltonian made by Swendsen [6], by comparing correlation functions calculated in different methods. His estimate, consisting of 17 coupling constants, combined with the majority-rule transformation, gave $\gamma/\nu = 1.9507(2)$, which is only about 0.5% from that accepted value.

Although the numbers given above give a good idea of the value of the IRG, they do not tell the whole story. In Fig. 1, we show a log-log plot of the susceptibility versus lattice size for both our two- and three-dimensional examples. In both cases, the linearity of the plots is striking, indicating the absence of corrections to scaling, even down to a 4^d lattice.

In Fig. 2, we show a log-log plot of the spin-spin correlation function, $\langle S_0 S_r \rangle$, as a function of separation, r, for the two-dimensional Ising model. Data for lattice sizes from 4×4 through 512×512 are shown by the curved dotted lines, one curve for each lattice size. One solid line goes through all the points corresponding to $L/2$ and another through the points corresponding to $L/4$. The dashed line, having slope -0.25, indicates the asymptotic behavior of the correlation function in the limit of an infinite system. The power law behavior in both cases is clearly seen, resulting in an estimate of $\eta = 0.250\,04(4)$.

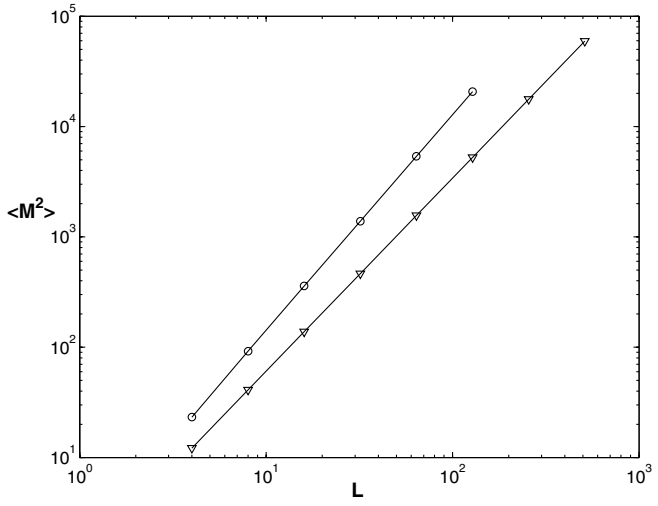

FIG. 1. A log-log plot of the linear size of the lattice L versus the average of the squared magnetization for the $d = 2$ and $d = 3$ Ising models. The line connecting the ∇ is obtained for the $d = 2$ fixed point using the seven-coupling Hamiltonian calculated by Swendsen. The line connecting the $\bigcirc$ is obtained for the 17-coupling Hamiltonian calculated by Swendsen to approximate the $d = 3$ fixed point. For both cases the RG transformation used is the majority rule for blocks of 2^d spins.

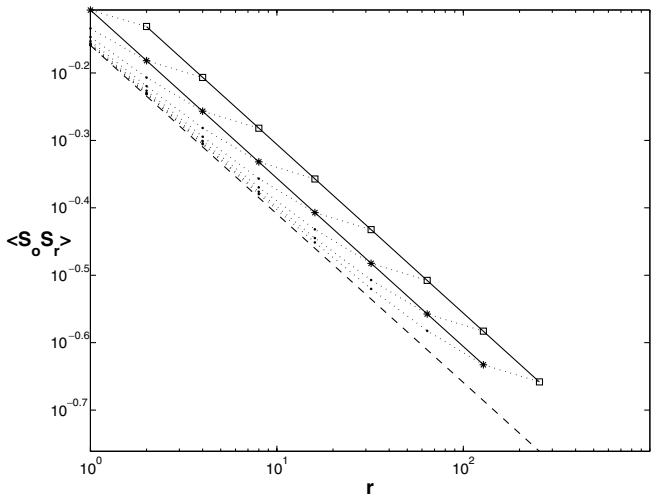

FIG. 2. A log-log plot of the spin-spin correlation function of distance r versus r, for the $d = 2$ Ising model with the majority rule, for lattice sizes $L = 4, 8, \ldots, 512$ where $r = 1, 2, \ldots, L/2$ using the seven-coupling Hamiltonian calculated by Swendsen. The line connecting the $\square$ connects all points for which $r = L/2$, and the $*$ are for $r = L/4$. The dashed line has the exact slope of -0.25.

In this Letter, we have presented a new approach to the renormalization group analysis of critical phenomena using Monte Carlo simulations. This method eliminates the problem of critical slowing down completely, for the same reasons that the coarse-to-fine equilibration of Brandt and Ron showed no critical slowing down. However, our approach also eliminates the difficulty that the coarse-to-fine equilibration method had in calculating appropriate Hamiltonians at every step.

Our results in two dimensions confirmed the validity of the basic method, giving excellent scaling and surprisingly accurate values for γ/ν and for η.

In three dimensions, an approximation to the FP Hamiltonian of the majority-rule RG using 17 couplings gives an error in γ/ν of only 0.5% in comparison with the best known values.

In both two and three dimensions, additional calculations that we do not have space to present here have confirmed the robustness of the method [10].

In future work, we will continue developing techniques for calculating improved estimations for the fixed point Hamiltonian to further improve the accuracy of the method, as well as applying this new approach to other models of critical phenomena.

In summary, we have developed a new way of using the renormalization group and Monte Carlo simulations to investigate critical behavior. Our approach does not suffer from critical slowing down and we hope that it will open the way to improved calculations of critical properties and insights into the structure of the renormalization group.

We thank R. Golubev for her helpful programming work. The research has been supported by Grant No. 295/01 from the Israel Science Foundation, U.S. Air Force Office of Scientific Research Contract No. F33615-97-D5405, U.S. Air Force EOARD Contract No. F61775-00-WE067, and by the Carl F. Gauss Minerva Center for Scientific Computation at the Weizmann Institute of Science.

[1] A. Compagner, A. Hoogland, and H.W. J. Blöte (unpublished).
[2] A. Brandt and D. Ron, J. Stat. Phys. **102**, 231 (2001).
[3] R. H. Swendsen, Phys. Rev. Lett. **42**, 859 (1979).
[4] R. H. Swendsen, Phys. Rev. Lett. **52**, 1165 (1984).
[5] R. H. Swendsen, Phys. Rev. B **30**, 3866 (1984).
[6] R. H. Swendsen, Phys. Rev. B **30**, 3875 (1984).
[7] H.W. J. Blöte, J. R. Heringa, A. Hoogland, E.W. Meyer, and T. S. Smit, Phys. Rev. Lett. **76**, 2613 (1996).
[8] R. Gupta and R. Cordery, Phys. Lett. **105A**, 415 (1984).
[9] D. Ron and R. H. Swendsen, Phys. Rev. E **63**, 066128 (2001).
[10] D. Ron, R. H. Swendsen, and A. Brandt (unpublished).