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Monte Carlo Renormalization Group

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A simplified method of applying a renormalization-group analysis to Monte Carlo simulations of general systems is presented and illustrated with applications to the Ising model and the three-state Potts model.

Two years ago, Ma[1] suggested combining Monte Carlo (MC) simulations of statistical-mechanical models[2] with a renormalization-group (RG) analysis of the critical properties.[3] The particular method which he suggested was based on a direct simulation of the fixed-point Hamiltonian, from which he calculated matrix elements for the linearized RG equations. The eigenvalues of these matrices then gave estimates of the critical exponents. Ma applied his method to the two-dimensional Ising model with encouraging results.

Ma's method has some drawbacks which have prevented its general application to problems of interest. The main difficulty was that the *direct* simulation of the fixed-point Hamiltonian involved a severe truncation in the number of coupling constants, while leaving a large parameter space to be scanned for the fixed point.

In this Letter, I would like to present a somewhat different approach that eliminates these difficulties: (1) It is only necessary to simulate the original Hamiltonian, *not* the fixed point or any renormalized Hamiltonian; (2) the truncation is small (and systematically improvable) if the range of interactions for the fixed-point Hamiltonian is small with respect to the lattice size; and (3) the parameter space to be scanned is only that of the original Hamiltonian. The result can be viewed as an extension of the standard methods of analyzing MC simulations that extracts useful information from correlation functions that are normally discarded. It can equally well be viewed as a systematically improvable real-space renormalization-group approximation that includes the effects of many interactions in the renormalized Hamiltonians.

Consider a lattice model in d dimensions with N^d sites. A "spin" σ_i (discrete or continuous) is associated with each site and the Hamiltonian has the general form

$$H = \sum_\alpha K_\alpha S_\alpha , \tag{1}$$

where each S_α is some combinations of the σ's that is translationally invariant subject to periodic boundary conditions. For example, H could be a two-dimensional Ising model, $\sigma_i = \pm 1$, and

$$S_1 = \sum_{\langle ij \rangle} \sigma_i \sigma_j ,$$

where the sum extends over all nearest-neighbor pairs. The RG transformation will, of course, generate effective interactions between more-distant neighbors as well as many-spin couplings.

Once a particular renormalization transformation, $H^{(n+1)} = R_b H^{(n)}$ (with scale factor b), is chosen, the asymptotic critical properties will be determined in the usual way by the eigenvalues of the linearized RG transformation matrix,

$T_{\alpha\beta}$*, in the vicinity of the fixed-point Hamiltonian, H*. Specifically,[3]

$$K_\alpha^{(n+1)} - K_\alpha^* = \sum_\beta T_{\alpha\beta}^*(K_\beta^{(n)} - K_\beta^*), \quad (2)$$

where

$$T_{\alpha\beta}^* = [\partial K_\alpha^{(n+1)}/\partial K_\beta^{(n)}]_{H^*} \quad (3)$$

and the eigenvalue equation is

$$\sum_\alpha \varphi_\alpha T_{\alpha\beta}^* = \lambda \varphi_\beta. \quad (4)$$

The critical exponents are obtained from the eigenvalues in the usual way [$\nu = \ln b/\ln\lambda_1^e$, $\eta = d + 2 - 2\ln\lambda_1^o/\ln b$, etc., where $\lambda_1^{e(o)}$ is the largest even (odd) eigenvalue].[3]

Note that, for these equations to be useful, the derivatives $\partial K_\alpha^{(n+1)}/\partial K_\beta^{(n)}$ must change slowly near the fixed point. To evaluate $T_{\alpha\beta}$*, it is therefore only necessary to calculate the derivatives somewhere in the "linear region," where they are essentially constant. Furthermore, only the eigenvalues have physical significance. The location of the fixed point (and even the space of Hamiltonians) depends on the choice of renormalization transformation and need not be calculated.

A sequence of approximations for $T_{\alpha\beta}$* can be obtained from an MC simulation of the system of interest at criticality. After the system has come to equilibrium, the simulation provides a sequence of configurations from which correlation functions can be calculated. Now apply an RG transformation to each configuration. For example, in the two-dimensional Ising model, one possibility is to divide the system into 3×3 blocks (scale factor $b=3$) and assign block spins of ±1 by majority rule. Such a procedure generates a sequence of configurations for the block spins. It is an important feature of the method that this sequence is equivalent to what would have been obtained if the *exact* RG transformation had been performed on H (a difficult calculation involving an extremely large number of coupling parameters) and the renormalized Hamiltonian had been simulated (also a difficult calculation). The RG transformation can, of course, be applied to the block spins repeatedly with the limitation that the last transformation leaves a lattice that is large with respect to the range of the corresponding renormalized Hamiltonian.

The chain rule

$$\frac{\partial\langle S_\gamma^{(n)}\rangle}{\partial K_\beta^{(n-1)}} = \sum_\alpha \frac{\partial K_\alpha^{(n)}}{\partial K_\beta^{(n-1)}} \frac{\partial\langle S_\gamma^{(n)}\rangle}{\partial K_\alpha^{(n)}}, \quad (5)$$

together with the identities

$$\frac{\partial\langle S_\gamma^{(n)}\rangle}{\partial K_\beta^{(n-1)}} = \langle S_\gamma^{(n)} S_\beta^{(n-1)}\rangle - \langle S_\gamma^{(n)}\rangle\langle S_\beta^{(n-1)}\rangle \quad (6)$$

and

$$\frac{\partial\langle S_\gamma^{(n)}\rangle}{\partial K_\alpha^{(n)}} = \langle S_\gamma^{(n)} S_\alpha^{(n)}\rangle - \langle S_\gamma^{(n)}\rangle\langle S_\alpha^{(n)}\rangle,$$

provides a direct way to calculate a sequence of approximations to $T_{\alpha\beta}$* as the renormalization transformation is iterated towards the fixed point.

The effective Hamiltonian, $H^{(n)}$, that corresponds to the nth iteration contains all interactions that fit onto a finite lattice with linear dimension N/b^n. (It is important that the smallest system considered is still large compared to the range of the fixed-point Hamiltonian so that any significant truncation is avoided.) However, it turns out that, for the evaluation of the eigenvalues by Eqs. (3)–(7), relatively few interactions need be considered explicitly. The effect on the eigenvalues and eigenvectors of including more interactions in the analysis can be investigated directly and the approximation can be improved

TABLE I. Eigenvalues and critical exponents obtained from an MC simulation of a two-dimensional Ising model using a 45×45 lattice with 9×10^4 MC steps/site. The second column gives the number of even interactions used in the RG analysis. The critical exponents are obtained from the eigenvalues in the usual way as described in Ref. 3.

Iteration	Even interactions	λ_1^e	ν	α	λ_1^o	δ	η	β	γ
1	1	2.817	1.061	−0.122	7.712	13.23	0.2812	0.1492	1.824
	2	2.887	1.036	−0.072				0.1457	1.781
	3	2.887	1.036	−0.072				0.1457	1.781
2	1	2.957	1.013	−0.026	7.835	14.85	0.2524	0.1278	1.770
	2	3.012	0.996	0.008				0.1257	1.741
	3	3.006	0.998	0.004				0.1259	1.744
Exact		3	1	0	7.8452	15	0.250	0.125	1.750

TABLE II. Eigenvalues (scale factor $b=2$) from an MC simulation of a two-dimensional, three-state Potts model on an 80×80 lattice with 3×10^4 MC steps/site.

Iteration	λ_1^e	λ_1^o
1	2.175±0.005	3.6517±0.0003
2	2.200±0.005	3.644±0.001
3	2.272±0.010	3.648±0.006
4	2.32	3.673

systematically, either by including more interactions in the analysis or by increasing the lattice size.

As a test of the method, I have applied it to the two-dimensional Ising model as mentioned above, analyzing up to three even interactions (nearest-neighbor, second-neighbor, and four-spin) and one odd interaction (magnetic field). The results are shown in Table I. They compare well with the results of other RG approximations and are superior to what has been achieved by standard MC analysis,[4] for which "the $d=2$ Ising lattice is, if anything, a rather unfavorable case."[5]

I have also used the method on the three-state Potts model,[6] which is of current interest because of its application to the behavior of krypton adsorbed on graphite.[7] The analysis used eight even and eight odd interactions. The results for the largest eigenvalue in each case (λ_1^e and λ_1^o) from a single simulation are shown in Table II.

The error estimates for the first three iterations are obtained by comparison with simulations of smaller lattices. It is difficult to give an error estimate for the fourth iteration with the present data. However, if we tentatively assign an error double that of the third iteration, we obtain $\nu=0.824(10)$, $\alpha=0.352(20)$, $\delta=15.26(60)$, $\eta=0.246(10)$, $\beta=0.101(6)$, and $\gamma=1.445(20)$, which agree quite well with series estimates[8-11] and are consistent with Suzuki's hypothesis[12] of "weak" universality in two dimensions ($\delta=15$, $\eta=\frac{1}{4}$).

In these examples I have taken advantage of knowing the exact critical temperatures. However, this knowledge is not necessary. MC simulation at temperatures above or below criticality clearly show the iteration towards high- or low-temperature fixed points and serve to locate the critical temperature self-consistently.

The Monte Carlo renormalization-group method also supplies information about the eigenvectors and other eigenvalues. This will be discussed elsewhere along with the convergence properties and the application of the method to other systems.

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Note added.—I would like to thank Dr. A. N. Berker for calling my attention to two additional estimates of the critical exponent α for the $d=2$, three-state Potts model: de Neef and Enting[13] have obtained $\alpha=0.42\pm0.05$ from series analysis; this value is considerably higher than that of Zwanzig and Ramshaw (Ref. 11). Bretz[14] has obtained an experimental value of $\alpha=0.36$ from a study of helium films on graphite, in excellent agreement with the MCRG results.

[1]S.-k. Ma, Phys. Rev. Lett. 37, 461 (1976).

[2]For a review, see K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 5b.

[3]For a review, see Th. Niemeijer and J. M. J. Van Leeuwen, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.

[4]Good accuracy has also been obtained from an MC simulation of the Ising model through an exploitation of scaling in RG form by Z. Friedman and J. Felsteiner, Phys. Rev. B 15, 5317 (1977). See also A. L. Lewis, Phys. Rev. B 16, 1249 (1977).

[5]K. Binder, Ref. 2, p. 41.

[6]R. B. Potts, Proc. Cambridge Philos. Soc. 48, 106 (1952).

[7]A. N. Berker, S. Ostlund, and F. A. Putnam, Phys. Rev. B 17, 3650 (1978).

[8]J. P. Straley and M. E. Fisher, J. Phys. A 6, 1310 (1973).

[9]I. G. Enting, J. Phys. A 7, 1617, 2181 (1964).

[10]D. Kim and R. I. Joseph, J. Phys. A 8, 891 (1975).

[11]The value of α is much larger than that given in Ref. 8 (0.05 ± 0.10), as it must be to satisfy the Rushbrooke inequality. It is also somewhat larger than the value of 0.296 ± 0.002 given by R. Zwanzig and J. D. Ramshaw, J. Phys. A 10, 65 (1977).

[12]M. Suzuki, Prog. Theor. Phys. 51, 1992 (1974).

[13]T. de Neef and I. G. Enting, J. Phys. A 10, 801 (1977).

[14]M. Bretz, Phys. Rev. Lett. 38, 501 (1977).