Optimization of Real-Space Renormalization-Group Transformations

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A general method for optimizing real-space renormalization-group transformations is presented. It is applicable to both spin systems and lattice gauge theories, with use of Monte Carlo computer simulations. It provides substantial improvement in the convergence of critical exponents for the $d=3$ Ising model.

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Although real-space renormalization-group (RG) methods have contributed much to our understanding of phase transitions,[1] their use has been limited by difficulties arising from the many parameters needed to describe the effective renormalized Hamiltonian completely. When truncation approximations are used, the neglect of all but a small number of coupling constants leads to uncertainties in the validity of the results. By combining the real-space renormalization-group formalism with Monte Carlo (MC) simulations, a relatively large number of operators can be used and assumptions concerning the renormalized couplings can be tested directly.[2-4] However, the convergence of the method and the required lattice size for the MC simulations depend on the number and range of the renormalized couplings.

Similarly, in MC studies of lattice gauge theories, the determination of the renormalization trajectory is greatly complicated by the generation of many effective coupling constants.[5-7]

In this Letter, I should like to present what I believe to be the first general method for optimizing real-space RG transformations to reduce, or even eliminate, these problems.

In earlier work, Witten and Prentis showed that certain values of the parameters in a truncation approximation gave particularly good results for the critical exponents.[8] In addition, they made the important observation that these values also produced especially small renormalized couplings beyond the nearest neighbors. However, they did not give a general method for optimization, but rather tried to "find accurate transformations empirically, and then look for criteria which characterize them."[8]

The first step in my procedure is to construct an RG transformation for which the renormalized Hamiltonian has specified properties. As a demonstration, I have explicitly constructed a local RG transformation that maps the nearest-neighbor Ising model at its critical point onto itself.

The nearest-neighbor Ising model is defined as

$$H = K_{nn} S_{nn} = K_{nn} \sum_{\langle ij \rangle} \sigma_i \sigma_j, \tag{1}$$

where $\sigma_i = +1$ or -1 and the sum is taken over nearest-neighbor pairs. In general, K_α will indicate the coupling parameter associated with an operator S_α, which is some combination of the spins.

Consider a general RG transformation

$$P'(\sigma') = \mathrm{Tr}_\sigma T(\sigma', \sigma) P(\sigma) = \mathrm{Tr}_\sigma \prod_j T_j(\sigma_j', \sigma) P(\sigma), \tag{2}$$

for which the renormalized spin on site j takes on the value σ_j' with probability

$$T_j(\sigma_j', \sigma) = Y_j^{-1} \exp[\sigma_j' \textstyle\sum_\alpha \rho_\alpha \hat{R}_{\alpha,j}(\sigma)] \tag{3}$$

and the normalization factor is

$$Y_j = \cosh[\textstyle\sum_\alpha \rho_\alpha \hat{R}_{\alpha,j}(\sigma)]. \tag{4}$$

The dependence of the renormalized spins on the local configurations of the original spins is contained in the functions $\hat{R}_{\alpha,j}(\sigma)$. For example, if $\hat{R}_{0,j}(\sigma)$ is the sum of spins in the block labeled j, the associated parameter is infinite, and there are no other contributions, then we have the usual majority rule.[1]

If MCRG simulations of a nearest-neighbor Ising model at its critical point are carried out with use of an RG transformation of this general form, and the renormalized Hamiltonian coincides with the nearest-neighbor critical point, the renormalized correlation functions will be the same as those of a nearest-neighbor model on the same size lattice. This can be checked by comparison of a direct evaluation of the correlation function with the result of using Callen's representation,[9-11]

$$\langle \tilde{S}_\alpha' \rangle = m_\alpha^{-1} \textstyle\sum_j \langle \hat{S}_{\alpha,j}' \tanh(K_c \hat{S}_{nn,j}) T(\sigma', \sigma) \rangle, \tag{5}$$

where the product $\sigma_j' \hat{S}_{\alpha,j}'$ is equal to the sum of all terms in S_α' containing σ_j', and m_α is a multiplicity factor to avoid double counting. For example, $\hat{S}_{nn,j}'$ is just the sum of the nearest neighbors of σ_j'. [Equation (5) can be easily generalized for models with different symmetry.[10,11]

By choosing the set $\{\rho_\alpha\}$ to make $\langle S_\alpha' - \tilde{S}_\alpha' \rangle = 0$,

the RG transformation can be optimized to make all renormalized coupling constants $\{K'_\alpha\}$ equal to zero except for the nearest-neighbor coupling.

Since the RG parameters only enter the expressions for the renormalized correlation functions through the weighting function $T(\sigma', \sigma)$, derivatives of the differences in the two expressions can be calculated from the MC simulation in a straightforward manner by differentiating Eqs. (3) and (4), allowing the optimal parameters to be found efficiently.

To illustrate this procedure, I have used an RG transformation based on the majority rule with scale factor $b = 2$. If the sum of the spins in a 2×2 block is nonzero, it determines the new spin to be $+1$ or -1 ($\rho_0 = \infty$). If the block sum is zero, the new spin is determined from Eqs. (3) and (4), with use of the sum of those neighboring renormalized spins that are uniquely determined by the majority rule. Different parameters correspond to different neighbors, and values found for the $d = 3$ Ising model are shown in Table I.

None of the optimized RG parameters is large, and they fall off rapidly with distance. Only one of the multispin terms seems to be significant, and it is far smaller than the nearest-neighbor contribution.

TABLE I. Parameters of an optimzed RG transformation for the nearest-neighbor $d = 3$ Ising model at the critical point. The second column gives the relative position of the neighbors contributing to $\hat{R}_{\alpha,j}(\sigma)$. The last three entries indicate contributions to $\hat{R}$ corresponding to the product of the spins at the indicated sites. These estimates were obtained from an MC simulation on a $16 \times 16 \times 16$ lattice, using 2.16×10^6 MC steps/site starting with a well-equilibrated configuration from older simulations, with data recorded every 20 MC steps/site. The numbers in parentheses indicate one-standard-deviation statistical error in the last digit.

ρ_α	Type
0.1592(6)	(100)
−0.0762(3)	(110)
−0.0473(3)	(111)
0.0396(5)	(200)
0.0025(3)	(210)
−0.0044(3)	(211)
0.0010(2)	(220)
−0.0019(2)	(221)
−0.0007(4)	(222)
0.0040(4)	(110) × (110) × (010)
−0.0201(4)	(100) × (010) × (001)
0.0021(3)	(111) × (110) × (001)

The success of the optimization has been checked by a direct computation of the renormalized coupling constants for the first two iterations.[11] The results for both iterations were consistent with the nearest-neighbor model within statistical errors of less than 0.0015 on the first and 0.007 on the second iteration for all seventeen coupling constants considered.

For the critical exponents, it is important to note that any local RG transformation should, in principle, lead to the correct values. If the optimized transformation has indeed mapped the critical point onto itself, there should also be no problem with convergence towards the fixed point in an MCRG calculation. Very small lattices could be used and the statistical errors would be greatly reduced.

This is particularly important for the $d = 3$ Ising model, for which extensive MCRG work has revealed a particularly slow convergence, requiring lattices of at least $64 \times 64 \times 64$ if a simple majority-rule transformation is used.[12,13]

As the data in Table II indicate, the optimization is still not perfect, but substantial progress has been made. The first iteration for y_{T1} is only about 2% below the best estimates of other methods, while the second iteration is already within the uncertainties of all other methods. Table II is to be compared with the sequence of estimates for y_{T1} of 1.425, 1.519, and 1.565 for the first three iterations with a simple majority rule.[13]

Table II also contains data for the leading irrelevant eigenvalue. Recent MCRG work by Pawley *et al.* using seven operators showed poor convergence for this eigenvalue and a deviation from the usually accepted value of about -0.8.[13] They attributed this to the small number of operators used and suggested that the inclusion of more terms would improve the convergence. Table II shows that this is indeed the case, and that MCRG results are consistent with those of other methods.

However, even though the convergence shown in Table II looks extremely good, the statistical errors for y_{T1} are small, and the values are those expected, systematic errors still have to be investigated and this calculation should be regarded as a feasibility study for future work. The values for the magnetic exponent in the first iterations turn out to be very sensitive to the RG parameters, and the calculation from which Table II was taken gave values of 2.502 and 2.500 on the first two iterations, instead of 2.485, as expected. Although this discrepancy is less than 1%, it could reflect a small error in the assumed values or a more fundamental problem, like the existence of a fixed point for imperfectly opti-

TABLE II. MCRG estimates for the leading thermal critical exponents of the nearest neighbor $d = 3$ Ising model from a simulation on a $16 \times 16 \times 16$ lattice. The RG transformation used older estimates for the optimized parameters that differ slightly from Table I. The simulation used 1.08×10^6 MC steps/site (starting from the last configuration of an earlier simulation), with data recorded every 20 MC steps/site. N_r is the number of RG steps and N_c is the number of couplings included in the analysis.

N_r	N_c	Y_{T1}	Y_{T2}	N_r	N_c	Y_{T1}	Y_{T2}
1	1	1.506(2)		2	1	1.519(9)	
	2	1.553(1)	−1.86(4)		2	1.588(8)	−2.01(4)
	3	1.558(1)	−1.56(2)		3	1.593(8)	−1.61(4)
	4	1.558(1)	−1.57(7)		4	1.590(8)	−1.65(10)
	5	1.556(2)	−1.04(5)		5	1.586(7)	−1.24(6)
	6	1.556(2)	−1.05(5)		6	1.585(7)	−1.33(7)
	7	1.556(2)	−1.14(3)		7	1.584(7)	−1.39(4)
	8	1.555(3)	−0.72(5)		8	1.584(9)	−0.74(6)
	9	1.556(3)	−0.73(4)		9	1.585(9)	−0.69(6)
	10	1.558(3)	−0.83(7)		10	1.586(9)	−0.74(7)
	11	1.558(3)	−0.76(8)		11	1.587(9)	−0.88(13)
	12	1.558(2)	−0.77(7)		12	1.585(9)	−0.88(14)
	13	1.558(2)	−0.75(10)		13	1.585(9)	−0.87(17)
	14	1.558(2)	−0.76(10)		14	1.585(9)	−0.87(17)
	15	1.558(2)	−0.76(10)		15	1.585(9)	−0.87(16)

mized transformations.[5]

It is perhaps surprising that so little freedom in the transformation is necessary to map the nearest-neighbor critical point onto itself. The success of the calculation suggests that it is possible to place the fixed point anywhere on the critical hypersurface. Note that this does not conflict with the association of irrelevant operators with corrections to scaling, since the amplitudes of the corrections do not have to vanish at a fixed point. In general, the amplitudes are determined by integrals along the trajectories away from the fixed point, rather than properties of the RG transformation at the fixed point. The small lattices required suggest that this approach can also be used in analytic work or different types of numerical calculations.[5]

In applications of the MCRG approach to lattice gauge theories, it is important to be able to follow the RG trajectory when the strength of the renormalized coupling is not known.[7] Hasenfratz *et al.* have already used optimized RG transformations in MCRG studies, where the optimization of a single parameter was done in perturbation theory.[14] Extending the above analysis to include the calculation of the renormalized coupling K_1',[11] while optimizing the RG transformation to set all other couplings equal to zero, would provide a systematic method for investigating one-parameter RG trajectories with use of MC simulations on small lattices. This procedure would also be applicable to the accurate location of critical points.

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