Another Monte Carlo Renormalization Group Algorithm
John P. Donohue
Department of Physics, University of California, Santa Cruz
Santa Cruz, CA 95064

Abstract
A Monte Carlo Renormalization Group algorithm is used on the Ising model to derive critical exponents and the critical temperature. The algorithm is based on a minimum relative entropy iteration developed previously to derive potentials from equilibrium configurations. This previous algorithm is modified to derive useful information in an RG iteration. The method is applied in several dimensions with limited success. Required accuracy has not been achieved, but the method is interesting.

Introduction
Monte Carlo Renormalization Group has been used with much success for over twenty-five years. The Large Cell Renormalization method calculates the renormalized parameters by renormalizing the system to a two spin system which can be solved exactly. Swendsen’s method avoids calculating the renormalized parameters by using a Taylor expansion of the Renormalization operator. Calculating several variances leads to a determination of the eigenvalues of the operator [8, 6, 4]. Ma’s method calculates the parameters in the Renormalized Hamiltonian using an analysis of the Monte Carlo dynamics [4, 5]. In our method, the parameters of the Renormalized Hamiltonian are derived using a minimum relative entropy iteration. The number of coupling parameters is controlled and error in the method can be estimated using usual statistical methods. The eigenvalues of the operator can be determined directly from the Renormalized Hamiltonian. This also allows the critical temperature to be directly calculated. Higher order coupling parameters can be included for an estimate of their effect.

Our Method
The following is based largely on an algorithm originally developed by reference [2]. The method is based on the following assumptions. The system is assumed to be in thermodynamic equilibrium and the energy can be written as a sum of terms which are products of parameters and functions of the configuration. $E(\Gamma, \vec{P}) = \sum_i p_i * h_i(\Gamma) = \vec{P} \cdot \vec{H}$ where $\Gamma$ represents the configuration of the system(s). $\vec{P} = \{p_i\}$ represents the set of parameters to be derived. In the case of the Ising Model, $E = -J \sum_{<ij>} s_i \cdot s_j - K \sum_i s_i$. In our notation, $h_1 = \sum_{<ij>} s_i \cdot s_j$, $p_1 = -J$, $h_2 = \sum_i s_i$ and $p_2 = -K$. 
The probability of a configuration, given parameters, is given by the Boltzmann distribution
\[ P(\Gamma | \vec{P}) = e^{-E(\Gamma, \vec{P})/kT}/Z = e^{(-E(\Gamma, \vec{P}) + F(\vec{P}))/kT}, \]
where \( Z(\vec{P}) = \sum_{\Gamma} \exp(-\beta E(\Gamma, \vec{P})) \) and \( F(\vec{P}) = -kT \ln(Z(\vec{P})) \).

If we are given the exact equilibrium conformation, \( \Gamma^* \), the maximum likelihood of parameter values are those values for which the probability, \( P(\Gamma^* | \vec{P}) \) is a maximum wrt \( \vec{P} \). Maximizing an exponential corresponds to maximizing the argument (ignoring the multiplicative constant \( \beta \)),
\[ -E(\Gamma^*, \vec{P}) + F(\vec{P}) = Q(\vec{P}). \]

This also corresponds to extremizing the entropy \( TS = E - F \).

Our method is basically the multi-dimensional form of Newton’s method for optimizing functions. Maximizing \( Q(\vec{P}) \), Newton’s Method is
\[ \vec{P}^{k+1} = \vec{P}^k - D^2(Q(\vec{P}^k))^{-1} \cdot D(Q(\vec{P}^k)) \] (1)
where \( (D^2)^{-1} \) represents the inverse Hessian matrix and \( D \) represents the gradient. In practice this is modified slightly,
\[ \vec{P}^{k+1} = \vec{P}^k + \epsilon(\Delta \vec{P}) \] (2)
where the use of \( \epsilon < 1 \) corresponds to the ”Damped Newton’s Method”.

Maximizing \( Q = -E + F \) wrt \( \vec{P} \) using statistical mechanical definitions leads to the following
\[ D(Q)_i = -h_i^* + < h_i > \] (3)
\[ D^2(Q)_{i,j} = \beta(< h_i > < h_j > - < h_i h_j >) = -\beta Cov(h_i, h_j) \] (4)

Resulting in the following iterative equation where \( VCM(\vec{H}) \) is the variance-covariance matrix of \( \vec{H} \)
\[ \Delta \vec{P} = kT * VCM(\vec{H})^{-1} \cdot (< \vec{H} > - \vec{H}^*) \] (5)
The method is easily generalized to a distribution of equilibrium configurations.
\[ \Delta \vec{P} = kT * VCM(\vec{H})^{-1} \cdot (< \vec{H} > - < \vec{H} >_{Prob(\Gamma)}) \] (6)
\(< ... > \) represents a Boltzmann average and \(< ... >_{Prob(\Gamma)} \) represents an average over the given distribution.

**Renormalization**

Renormalization can be described as an operator acting on the original Hamiltonian to create a Renormalized Hamiltonian. Linearizing the operator near the fixed point, relevant eigenvalues can be isolated. By examining the plot of renormalized vs original parameters, the eigenvalues can be determined. The eigenvalues \( \lambda_i \), correspond to the slope of these lines. With the usual approximations, the exponents can be calculated, \( \nu_i = \ln(b)/\ln(\lambda_i) \). The critical temperature can be determined by calculating the intersection of the derived thermal coupling parameters and the line \( y=x \). Flow diagrams could easily be extracted, although they are not done in this study.
Using Renormalization notation, the reduced hamiltonian for the Ising model is given below.

\[ H_r = -\frac{H}{kT} \quad (7) \]

\[ H_r = K_0 \Sigma s_i + K_1 \Sigma_{nn} s_is_j + K_2 \Sigma_{nnn} s_is_j + K_4 \Sigma_{square} s_is_js_j + \ldots \quad (8) \]

Applying the algorithm to Renormalization requires an outer iteration over a parameter (ie \( K_i \) for some \( i \)) while other parameters remain fixed. The original system(s) is brought to equilibrium at some fixed values for all parameters. The renormalized system(s) is created from this original system. The above iteration represented by equations 1, 2 and 5 can be carried out on large number of lattices simultaneously to determine what values of parameters would lead to this renormalized system. As a parameter is varied the corresponding eigenvalues and critical exponents can be derived. The method is simpler to apply if the renormalization method is not a quasi-linear method [3]. Majority rule renormalization is used in all of the following.

2-D Ising Model

The algorithm was attempted on a 2-D Ising model. Exponents and critical temperature are known from the original solution by Onsager [7, 1].

\( \nu = 1 \), \( \theta = 8/15 \) and \( T_{\text{critical}} = 2.269 \)

2D Ising Model Thermal Coupling Exponent

The thermal eigenvalue can be determined by varying the ratio of \( J/kT \) through the critical value at zero field. The corresponding exponent, in terms of correlation length and reduced temperature, is

\[ \xi \propto |t|^{-\nu} \quad (9) \]

The renormalized parameters were calculated as per the above algorithm. Figure 1 shows several runs of various lattice sizes and number. The slopes, exponents and critical temperatures are shown in table 1.

| Size | Slope | \( \nu = \ln 2/ \ln(\text{slope}) \) | Intercept | \( T_{\text{critical}} \) |
|------|-------|---------------------------------|-----------|---------------------|
| 8    | 1.96 ± 0.04 | 1.03 ± 0.03 | 0.43 ± 0.02 | 2.23 ± 0.14 |
| 16   | 1.99 ± 0.02 | 1.01 ± 0.01 | 0.44 ± 0.01 | 2.25 ± 0.07 |
| 32   | 2.02 ± 0.03 | 0.99 ± 0.02 | 0.45 ± 0.01 | 2.27 ± 0.08 |
| 32(W) | 1.95 ± 0.01 | 1.03 ± 0.01 | 0.42 ± 0.01 | 2.26 ± 0.06 |
| 64(W) | 1.98 ± 0.02 | 1.01 ± 0.02 | 0.43 ± 0.01 | 2.28 ± 0.07 |

Table 1: Calculation of 2-D Ising model thermal coupling exponent. Exact value is \( \nu = 1 \) and \( T_{\text{critical}} = 2.269 \)
Figure 1: Plot of Renormalized parameter $K_1'$ (Y-axis) vs $K_1$ (X-axis) for 2-D Ising model. Intersection of the line $y=x$ with the data corresponds to the fixed point. Error bars are included on the plot but are on the scale of the size of the points.
Magnetic eigenvalue

The other exponent and eigenvalue can be determined by fixing $J/kT$ at approximately the critical value and varying the field parameter through zero. The corresponding exponent, in terms of correlation length and field, is

$$\xi \propto |K|^{-\theta}$$

(10)

$K$ represents the external field. The renormalized parameters were calculated as per the above algorithm. Figure 2 shows data runs over a large variation in field parameter. The critical region, near zero field, shows a more linear relationship as shown in figure 3. Least squares best fit to a straight line was done on this central region. The results are shown in table 2.

Figure 2: Plot of Renormalized magnetic parameter/kT (Y-axis) vs Original magnetic parameter/kT (X-axis) for 2-D Ising model near the critical temperature. 4000 MC steps per site were used. Data is from systems with a.)16x16,n=1024 b.)8x8,n=1024.

| Size | Slope   | $\theta = \ln 2 / \ln(\lambda)$ |
|------|---------|---------------------------------|
| 8    | 3.63 ± 0.48 | 0.54 ± 0.06                     |
| 16   | 3.68 ± 0.16 | 0.53 ± 0.02                     |

Table 2: Calculation of magnetic exponent for 2-D Ising model. Exact value is $\theta = 8/15 = 0.53$
Figure 3: Plot of Renormalized magnetic parameter/kT (Y-axis) vs Original magnetic parameter/kT (X-axis) for 2-D Ising model near the critical temperature.
3D Ising Model Eigenvalues

The algorithm was applied to the 3D and 4D Ising model with encouraging results, even on small lattice sizes. Approximate exponents for 3D are known from several sources. Reviews are given by references [1, 4].

Size | $\text{Slope} = a$ | $\nu = \ln 2 / \ln(slope)$ | Intercept = $b$ | $T_{\text{critical}} = (1 - a) / b$
--- | --- | --- | --- | ---
4   | $3.02 \pm 0.07$ | $0.63 \pm 0.01$ | $0.44 \pm 0.02$ | $4.59 \pm 0.17$
32  | $3.40 \pm 0.09$ | $0.57 \pm 0.01$ | $0.53 \pm 0.02$ | $4.53 \pm 0.24$

Table 3: Calculation of thermal coupling exponent for 3-D Ising model. Approximate value is $\nu \approx 0.63$ and $T_{\text{critical}} \approx 4.52$.

| Size | $\text{Slope}$ | $\theta = \ln 2 / \ln(slope)$ | Intercept = $b$ |
--- | --- | --- | ---
4   | $6.3 \pm 0.3$ | $0.38 \pm 0.01$ | ---

Table 4: Calculation of magnetic exponent for 3-D Ising model. Expected value $\theta \approx 0.40$
4D Ising Model - Mean Field Theory Exponents

| Size | Slope = a | $\nu = \ln 2 / \ln(slope)$ | Intercept = b | $T_{critical} = (1 - a) / b$ |
|------|-----------|----------------------------|--------------|-----------------|
| 4    | 4.3 ± 0.1 | 0.48 ± 0.04                | 0.48 ± 0.02  | 6.88 ± 0.5      |

Table 5: Calculation of thermal coupling exponent for 4-D Ising model. Exact values are $\nu = 0.5$ and $T_{critical} = 6.68$.

| Size | Slope     | $\theta$ exact |
|------|-----------|----------------|
| 4    | 10.2 ± 0.8| 0.333...       |

Table 6: Calculation of magnetic exponent for 4-D Ising model. Exact value is $\theta = 1/3$. 
Conclusion

Much higher precision and accuracy is required to compare with current estimates of exponents, but the derived exponents match reasonably well with expected values. Improvement is expected with larger lattices and more systems, perhaps with more clever averaging methods. The effect of critical slowing down has not been thoroughly investigated. The algorithm has several advantages over other algorithms. The number of coupling parameters is kept the same from original system to the renormalized system with minimum relative entropy derived values for the renormalized parameters. This seems more consistent than an arbitrary cutoff in parameter space. The renormalized parameters are directly calculated, unlike other algorithms. By changing the parameter of the outer iteration, all exponents can be magnified and derived. If flow diagrams are desired, the algorithm could be easily modified to provide them. The error in the calculated exponents can be derived through usual statistical properties.

Acknowledgments

J Deutsch, AP Young, Lik Wee Lee, Leif Poorman, Stefan Meyer, TJ Cox, B Allgood, D Doshay, Hierarchical Systems Research Foundation

References

[1] R.J. Creswick, H.A. Farach, and C.P. Poole Jr. Introduction to Renormalization Group Methods in Physics. John Wiley and Sons, 1992.

[2] JM Deutsch and T Kurosky. Design of force fields from data at finite temperature. arXiv.org:cond-mat/9609097, 1996.

[3] M.E. Fisher. Lecture Notes in Physics, 186, 1983.

[4] D.P. Landau and K. Binder. A Guide to Monte Carlo Simulations in Statistical Physics. Cambridge University Press, 2000.

[5] S.K. Ma. Phys. Rev. Lett., 37, 1976.

[6] M.E.J. Newman and G.T. Barkema. Monte Carlo Methods in Statistical Physics. Clarenden Press, Oxford, 1999.

[7] L Onsager. Phys. Rev., 65, 1944.

[8] R.H. Swendsen. Topics in Current Physics: Real-Space Renormalization, 30, 1982.