MONTE CARLO RENORMALIZATION GROUP

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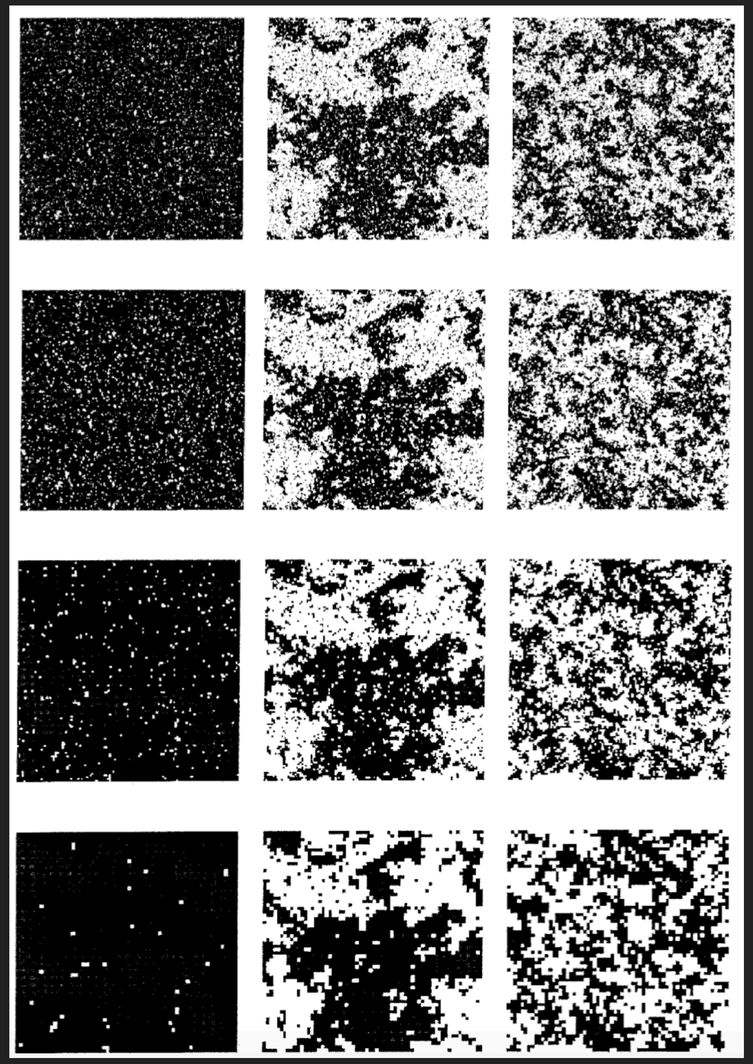
DECEMBER 18, 2020

OUTLINE

- Review of key concepts
- Swendsen's MCRG method
  - Calculate critical coupling
  - Extract critical exponents
  - Monte Carlo simulation
- Example: 2D Ising model



Landau and Binder, A Guide to Monte Carlo Simulations in Statistical Physics (2005).

REVIEW OF KEY CONCEPTS

- Ising-type Hamiltonian:

$$\mathscr{H} = \beta H = \sum_{\alpha} K_{\alpha} S_{\alpha}$$

- Recall:

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad J > 0, \quad \Longrightarrow \quad K_1 = -\beta J, \quad S_1 = \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

- Starting Hamiltonian:

$$\mathscr{H}^{(0)} = K_1^{(0)} S_1^{(0)}, \quad K_{\alpha} = 0 \quad \forall \quad \alpha > 1$$

REVIEW OF KEY CONCEPTS

- Starting Hamiltonian:

$$\mathscr{H}^{(0)} = K_1^{(0)} S_1^{(0)}, \quad K_\alpha = 0 \quad \forall \quad \alpha > 1$$

- After n RG transformations:

$$\mathscr{H}^{(n)} = \sum_\alpha K_\alpha^{(n)} S_\alpha^{(n)}$$

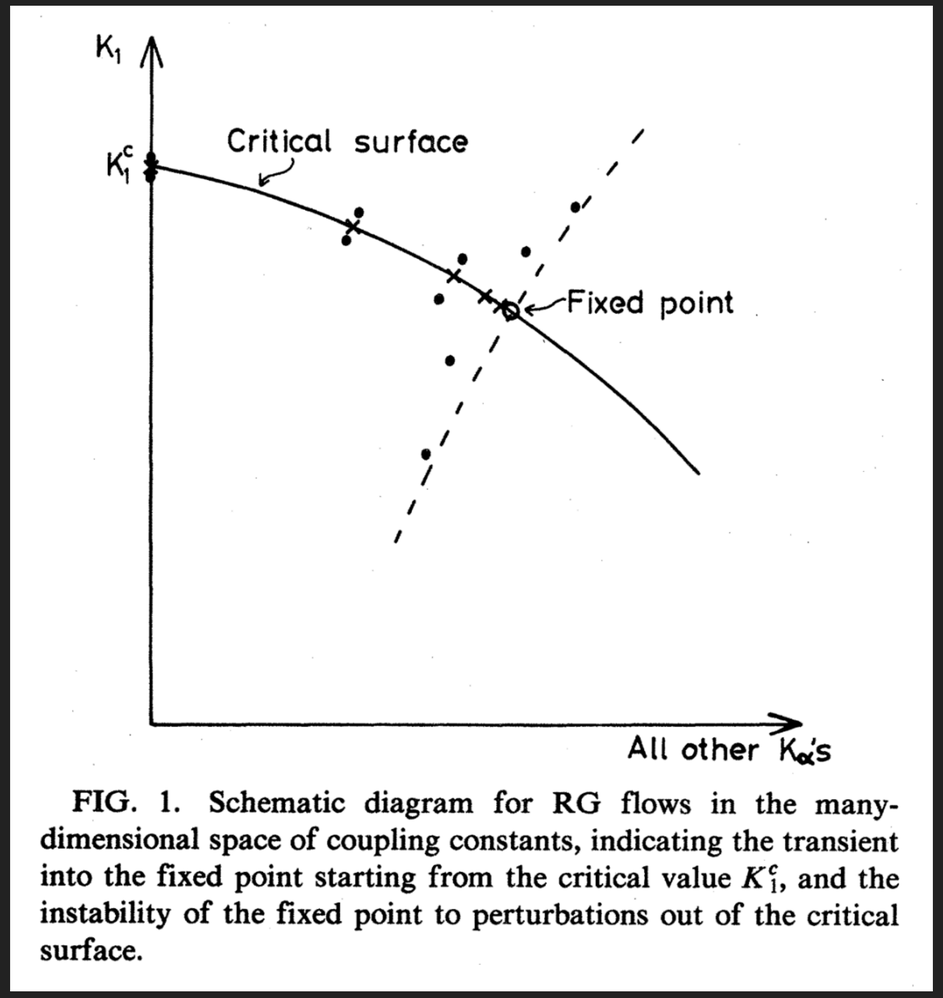


FIG. 1. Schematic diagram for RG flows in the many-dimensional space of coupling constants, indicating the transient into the fixed point starting from the critical value K_1^c, and the instability of the fixed point to perturbations out of the critical surface.

Pawley et al., Phys. Rev. B 29, 4030 (1984)

REVIEW OF KEY CONCEPTS

- Choose a renormalization transformation (with scale factor b):

$$\mathscr{H}^{(n+1)} = R_b \mathscr{H}^{(n)}$$

- Linearize transformation about fixed-point Hamiltonian $\mathscr{H}^*$:

$$\delta K_\alpha^{(n+1)} = T^*_{\alpha\beta} \delta K_\beta^{(n)}, \text{ where } T^*_{\alpha\beta} = \left. \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}} \right|_{\mathscr{H}=\mathscr{H}^*}$$

- Goal: Calculate the eigenvalues of $T^*_{\alpha\beta}$.

REVIEW OF KEY CONCEPTS

- External magnetic field is zero at the critical point.
- $T^*_{\alpha\beta}$ decouples into a block diagonal form.

$$\lambda_1^{(e)} = \text{largest eigenvalue of } T^{*(e)}_{\alpha\beta} \implies \lambda_1^{(e)} = b^{y_t}$$
$$\lambda_1^{(o)} = \text{largest eigenvalue of } T^{*(o)}_{\alpha\beta} \implies \lambda_1^{(o)} = b^{y_h}$$

- Critical exponents written in terms of RG exponents y_t, y_h.

REVIEW OF KEY CONCEPTS

- For d dimensions:

$$\alpha = 2 - \frac{d}{y_t}, \quad \beta = \frac{d - y_h}{y_t}, \quad \gamma = \frac{2y_h - d}{y_t}, \quad \delta = \frac{y_h}{d - y_h}, \quad \eta = d + 2 - 2y_h, \quad \nu = \frac{1}{y_t}$$

- For 2D Ising model:

$$y_t = 1, \quad y_h = \frac{15}{8} \quad \Longrightarrow \quad \alpha = 0, \quad \beta = \frac{1}{8}, \quad \gamma = \frac{7}{4}, \quad \delta = 15, \quad \eta = \frac{1}{4}, \quad \nu = 1$$

MA'S METHOD

- First MCRG approach (1976).
- Basic idea:
  - Explicitly flow towards fixed point in truncated coupling space.
  - Construct $T^*_{\alpha\beta}$ directly from renormalized Hamiltonian.
- Drawbacks:
  - Truncation errors accumulate quickly.
  - Monte Carlo simulation involves many couplings.

MA'S METHOD

Approximate K^*

Equilibrate spins at K^*

Sample configurations at K^*

Calculate $T^*_{\alpha\beta}$ $\rightarrow$ critical exponents

SWENDSEN'S METHOD

Approximate K_1^c

Equilibrate spins at $K = (K_1^c, 0)$

Sample configurations at K

Apply n RG transformations

Calculate $T^*_{\alpha\beta}$ $\rightarrow$ critical exponents

SWENDSEN'S METHOD – CALCULATING CRITICAL COUPLING

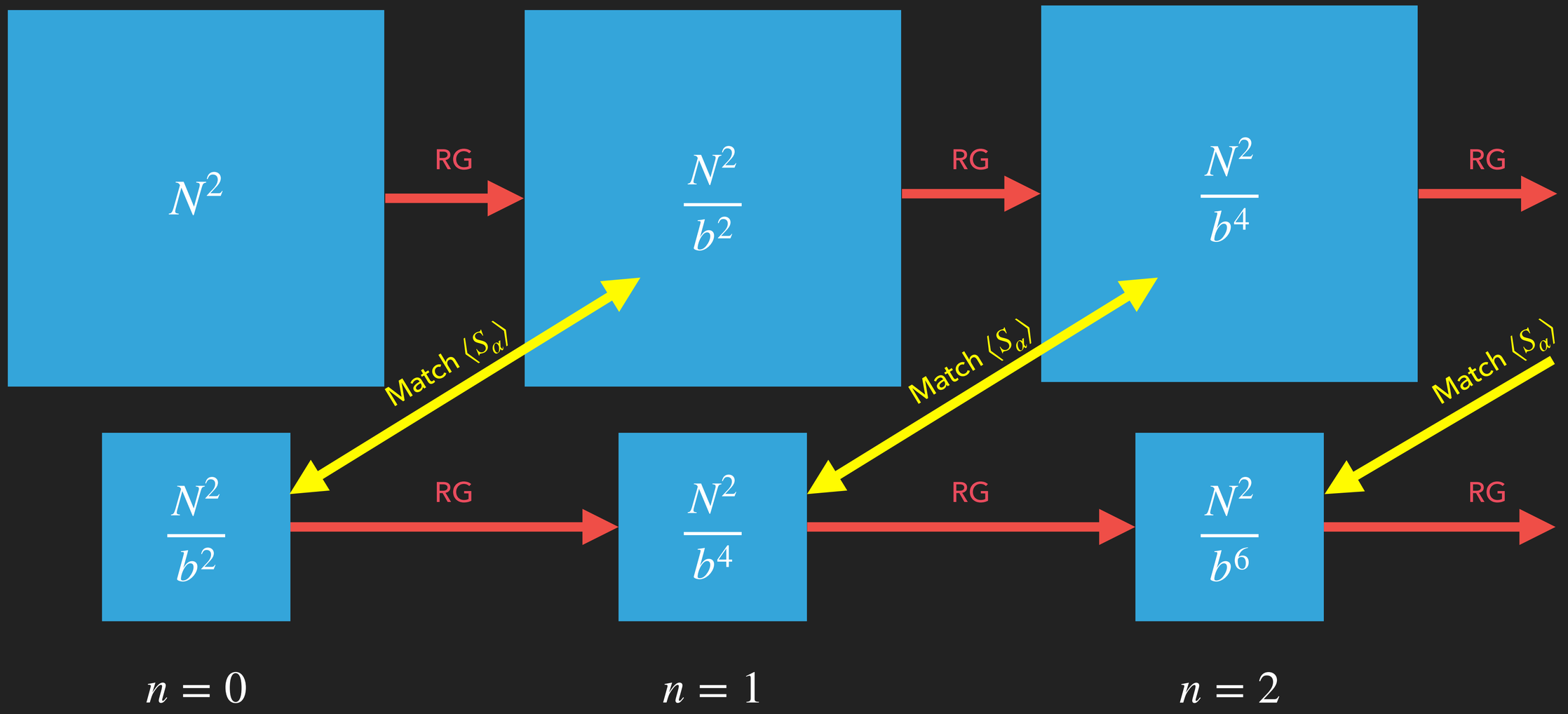
- Match correlation functions for transformed and untransformed systems.
- Cancel unknown finite size effects by comparing lattices of different sizes but the same number of lattice sites:

$$\left\langle S_\alpha^{(n+m)} \right\rangle_L = \left\langle S_\alpha^{(n)} \right\rangle_S ,$$

  where $L = N^2$ and $S = N^2/b^{2m}$.

- Most effective for large lattices and large n.

SWENDSEN'S METHOD – CALCULATING CRITICAL COUPLING



SWENDSEN'S METHOD – CALCULATING CRITICAL COUPLING

- Linear approximation:

$$\left\langle S_\alpha^{(n+m)} \right\rangle_L - \left\langle S_\alpha^{(n)} \right\rangle_S = \left[\frac{\partial \langle S_\alpha^{(n)} \rangle_L}{\partial K_1^{(0)}} - \frac{\partial \langle S_\alpha^{(n)} \rangle_S}{\partial K_1^{(0)}} \right] \delta K_1^{(0)} ,$$

where

$$\frac{\partial \langle S_\alpha^{(n)} \rangle}{\partial K_1^{(0)}} = \left\langle S_\alpha^{(n)} S_1^{(0)} \right\rangle - \left\langle S_\alpha^{(n)} \right\rangle \left\langle S_1^{(0)} \right\rangle .$$

SWENDSEN'S METHOD – CALCULATING CRITICAL EXPONENTS

- Chain rule and invert:

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}} = \frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}} \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}} \implies T_{\alpha\beta}^{(n)} = \left[\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}} \right]^{-1} \frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}}$$

- Calculate derivatives using MC samples:

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}} = \langle S_\gamma^{(n+1)} S_\alpha^{(n+1)} \rangle - \langle S_\gamma^{(n+1)} \rangle \langle S_\alpha^{(n+1)} \rangle$$

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

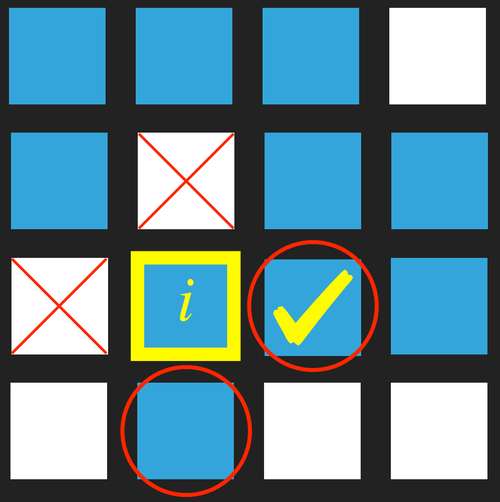
SWENDSEN'S METHOD – CALCULATING CRITICAL EXPONENTS

- Need to construct both even and odd blocks for β and γ.
- Only need even block for α and ν.
- Only need odd block δ and η.
- For 2D Ising model example, consider nearest-neighbor and next-nearest-neighbor spin interactions only.
- Again, calculation of $T_{\alpha\beta}^{(n)}$ most accurate for large lattices and large n.

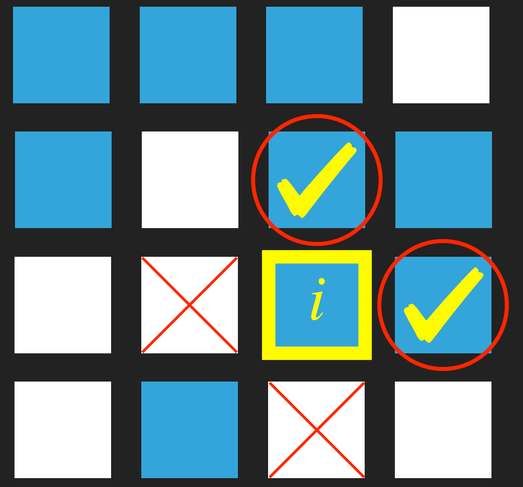
MONTE CARLO SIMULATION

- At criticality, correlation length diverges.
- Standard Metropolis updates are too local to efficiently simulate Ising system.
- Need cluster algorithms:
  - Swendsen-Wang algorithm
  - Wolff algorithm
- Wolff update has a larger probability of flipping a larger cluster of spins compared to a Swendsen-Wang update.

WOLFF ALGORITHM



1. Choose random site i to add to the initially empty cluster.
2. Search through nearest neighbor sites j. If $\sigma_i = \sigma_j$, add site j to the cluster with probability $P = 1 - e^{2K_1}$.
3. Flip spin at site i and remove from the cluster.
4. If cluster is still empty, go back to step 1.
5. If cluster is not empty, repeat steps 2-5 until cluster stops growing.



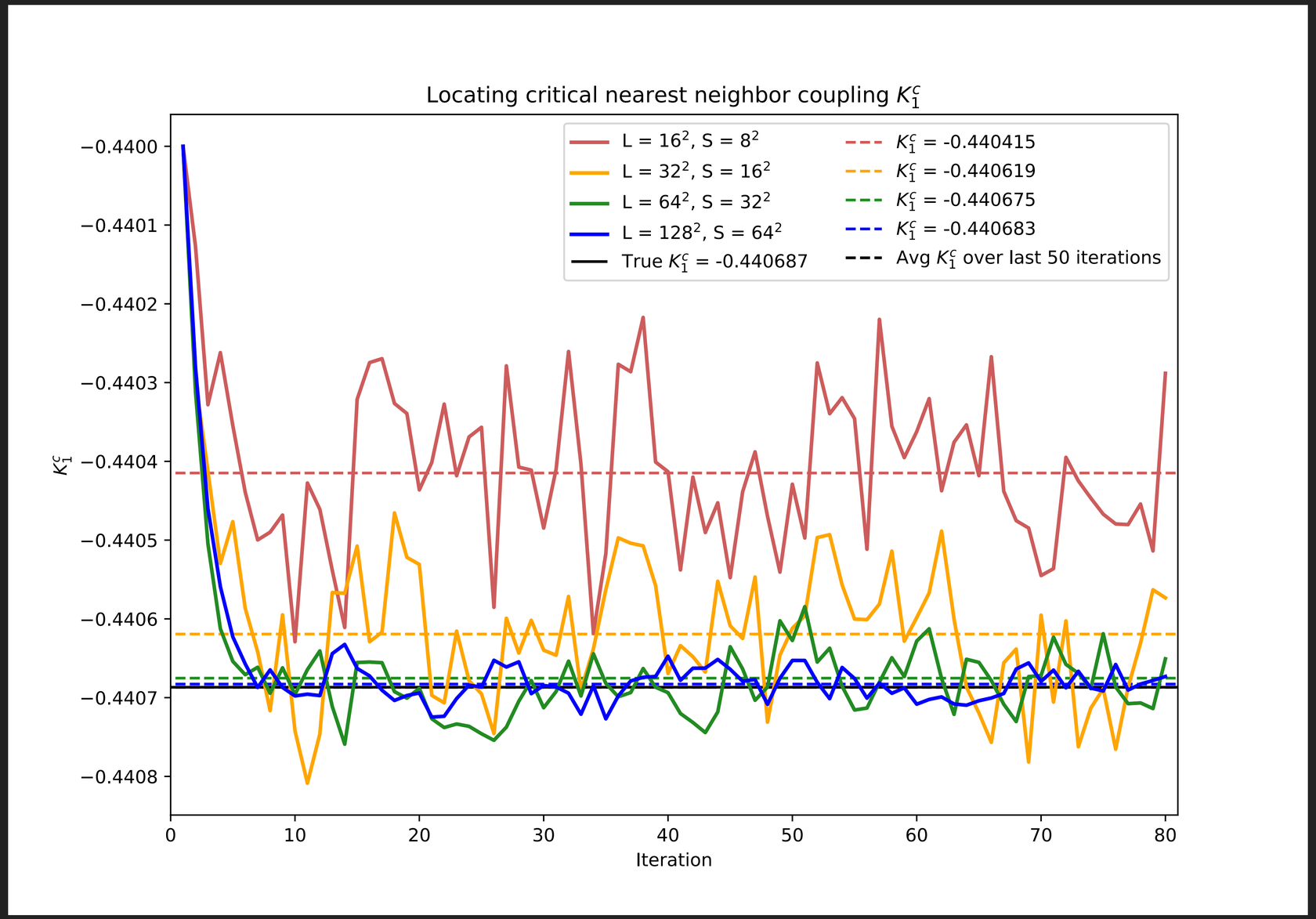
EXAMPLE: 2D ISING MODEL

- Simple implementation:
  - Sample from pure nearest-neighbor Ising Hamiltonian using Wolff algorithm.
  - Majority-rule block spin transformation with scale factor b.
  - Use only nearest-neighbor spin correlation functions to tune K_1^c.
  - Use nearest-neighbor and next-nearest-neighbor spin correlations to construct truncated $T_{\alpha\beta}^{(e)}$.
  - Extract largest even eigenvalue $\lambda_1^{(e)}$ and calculate $\nu = \ln b / \ln \lambda_1^{(e)}$.

EXAMPLE: 2D ISING MODEL

- 1E4 samples during equilibration.
- 1E6 samples for locating critical coupling.
- 1E7 samples for calculating critical exponent.
- Calculated ν at $K_1^c(N)$ and $K_1^c(N \to \infty)$.
- Recall Onsager's solution:

$$T_c = \frac{2J}{\ln(1+\sqrt{2})} \implies K_c \equiv K_1^c(N \to \infty) = -\frac{\ln(1+\sqrt{2})}{2} \approx -0.440687$$


Locating critical nearest neighbor coupling K_1^c
L = 16^2, S = 8^2
L = 32^2, S = 16^2
L = 64^2, S = 32^2
L = 128^2, S = 64^2
True K_1^c = -0.440687
K_1^c = -0.440415
K_1^c = -0.440619
K_1^c = -0.440675
K_1^c = -0.440683
Avg K_1^c over last 50 iterations
−0.4400
−0.4401
−0.4402
−0.4403
−0.4404
−0.4405
−0.4406
−0.4407
−0.4408
K_1^c
0
10
20
30
40
50
60
70
80
Iteration

RESULTS

- First iteration of locating critical coupling K_1^c from starting value $K_1 = -0.44$ for various blocking levels and lattice sizes:

n	N = 16	N = 32	N = 64	N = 128
0	-0.4420811188	-0.4417429398	-0.4415445759	-0.4413292658
1	-0.4404791358	-0.4404577112	-0.4404935597	-0.4404266727
2	-0.4401272033	-0.4402638848	-0.4403468642	-0.4403131062
3	-	-0.4402975527	-0.4403307834	-0.4403016019
4	-	-	-0.4403116430	-0.4402985574
5	-	-	-	-0.4402807798

BENCHMARK

Table 9.1 *Variation of the thermal eigenvalue exponent for the Ising square lattice with the number of couplings N_c, the number of iterations N_r, and for different lattice sizes. From Swendsen (1982).*

N_r	N_c	$L = 64$	$L = 32$	$L = 16$
1	1	0.912(2)	0.904(1)	0.897(3)
1	2	0.967(3)	0.966(2)	0.964(3)
1	3	0.968(2)	0.968(2)	0.966(3)
1	4	0.969(4)	0.968(2)	0.966(3)
2	1	0.963(4)	0.953(2)	0.937(3)
2	2	0.999(4)	0.998(2)	0.993(3)
2	3	1.001(4)	1.000(2)	0.994(3)
2	4	1.002(5)	0.998(2)	0.984(4)
3	1	0.957(2)	0.936(3)	0.921(5)
3	2	0.998(2)	0.991(3)	1.013(4)
3	3	0.999(2)	0.993(3)	1.020(3)
3	4	0.997(2)	0.987(4)	...

Landau and Binder, A Guide to Monte Carlo Simulations in Statistical Physics (2005).

RESULTS

- Critical exponent ν for $N = 16,\ 32$ and various blocking levels at known critical coupling K_1^c and calculated critical coupling $K_1^c(N)$:

n	N = 16 @ $K_1^c(N)$	N = 16 @ K_1^c	N = 32 @ $K_1^c(N)$	N = 32 @ K_1^c
0	1.0366474702	1.0371936855	1.0359594271	1.0364461518
1	1.0055084088	1.0058615220	1.0030411491	1.0024276306
2	0.9850458988	0.9832937022	1.0042751683	1.0040962187
3	-	-	0.9833658883	0.9817702370

RESULTS

- Critical exponent ν for $N = 64,\ 128$ and various blocking levels at known critical coupling K_1^c and calculated critical coupling $K_1^c(N)$:

n	N = 64 @ $K_1^c(N)$	N = 64 @ K_1^c	N = 128 @ $K_1^c(N)$	N = 128 @ K_1^c
0	1.0340840722	1.0356603405	1.0343762634	1.0349921920
1	1.0013550363	1.0025377191	1.0018397044	1.0006737634
2	1.0021687106	1.0029573471	1.0019303651	1.0022232598
3	1.0029619937	1.0039006140	1.0025651221	1.0023411428
4	0.9820802731	0.9819506190	1.0035789853	1.0040042374
5	-	-	0.9814148379	0.9819137809

CONCLUSION

- Swendsen's MCRG method can efficiently extract critical exponents, even in an aggressively truncated coupling space.
- Truncation errors are small and systematically improvable by including higher order couplings and by simulating larger lattices.
- Computational costs are kept low by only requiring the simulations of pure nearest-neighbor Ising systems.

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QUESTIONS?