Generating configurations of increasing lattice size with machine learning and the inverse renormalization group

Dimitrios Bachtis

In one sentence:

We can use the inverse renormalization group to construct configurations for lattice volumes that have not yet been accessed by dedicated supercomputers.

Disclaimers

1. I am not going to talk about groups or semi-groups, see:

Inverse Monte Carlo Renormalization Group Transformations for Critical Phenomena,
D. Ron, R. Swendsen, A. Brandt, Phys. Rev. Lett. 89, 275701 (2002)

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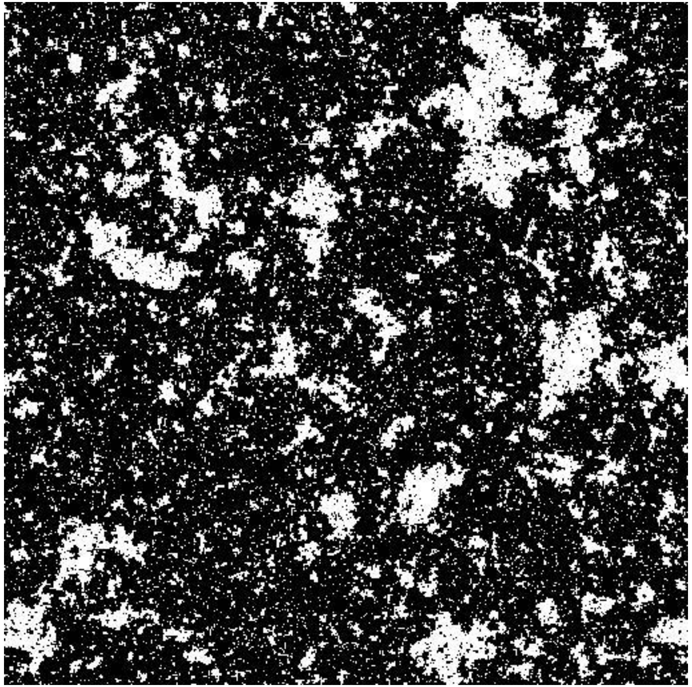
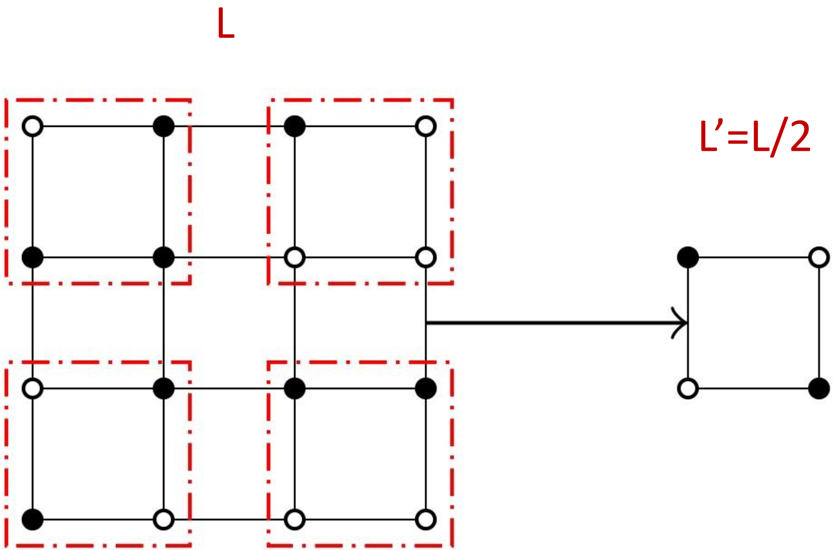
3. Numerical exactness is a special case in the Monte Carlo renormalization group.

Standard renormalization group

L

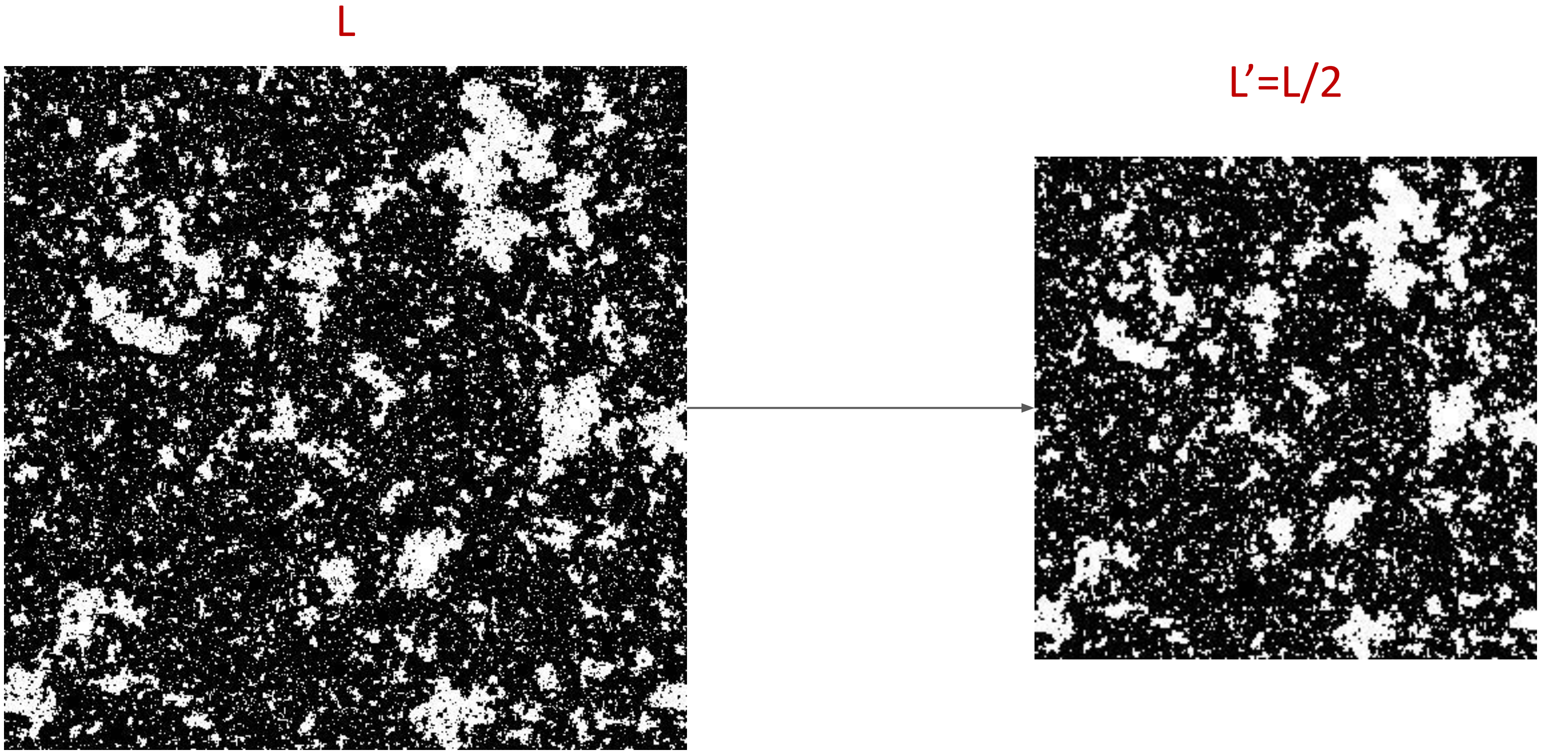


Standard renormalization group



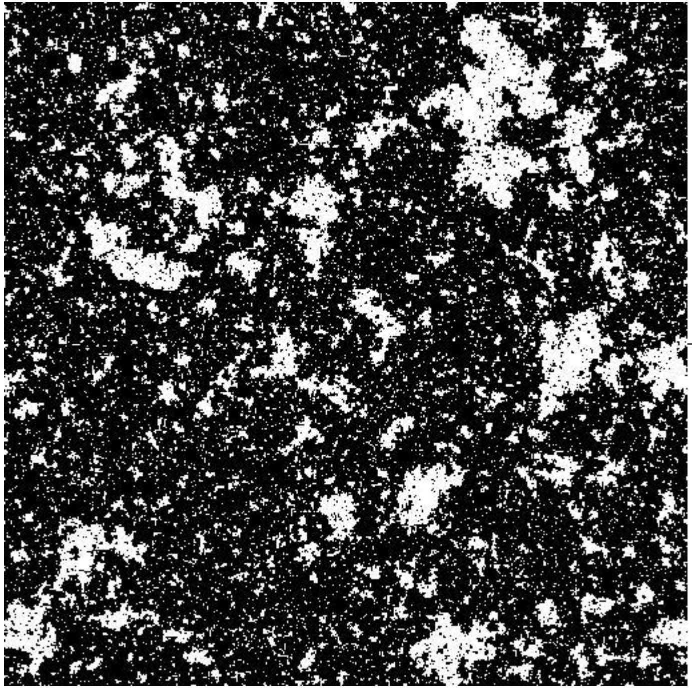
Spin blocking transformation with a rescaling factor of b=2 and the majority rule

Standard renormalization group

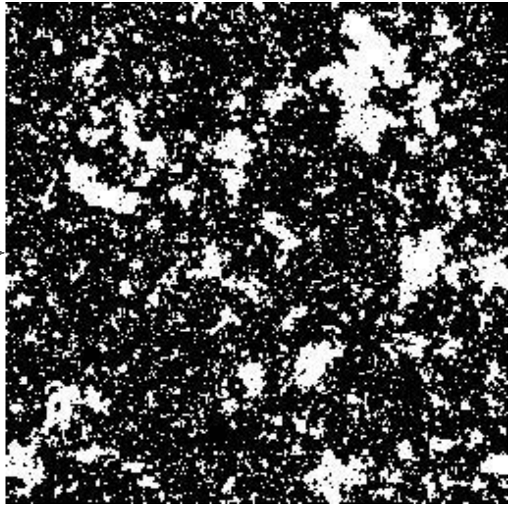


Standard renormalization group

L, ξ

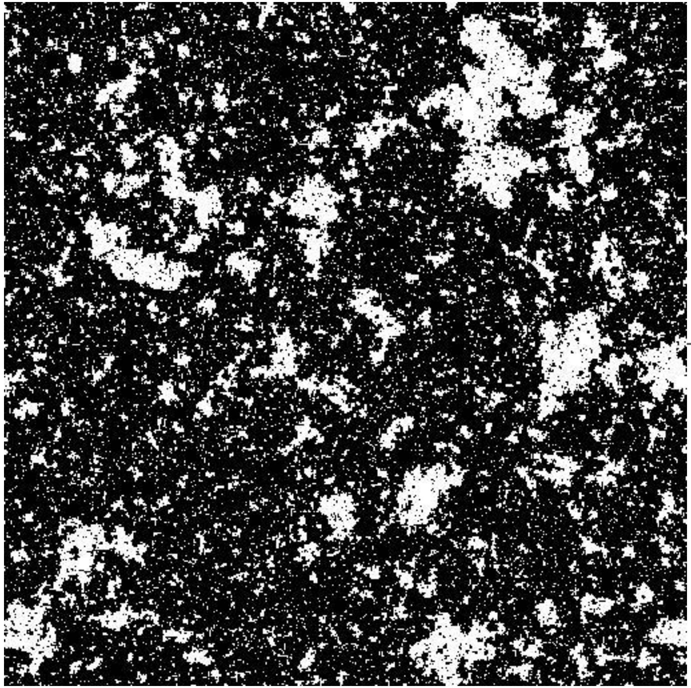


L'=L/2, ξ'=ξ/2

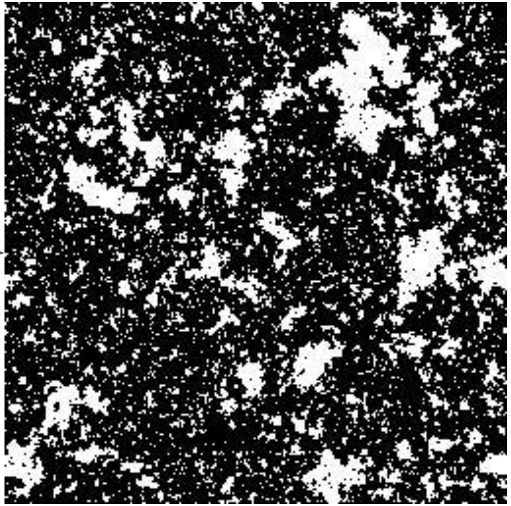


Standard renormalization group

L, ξ, β



L’=L/2, ξ’=ξ/2, β’



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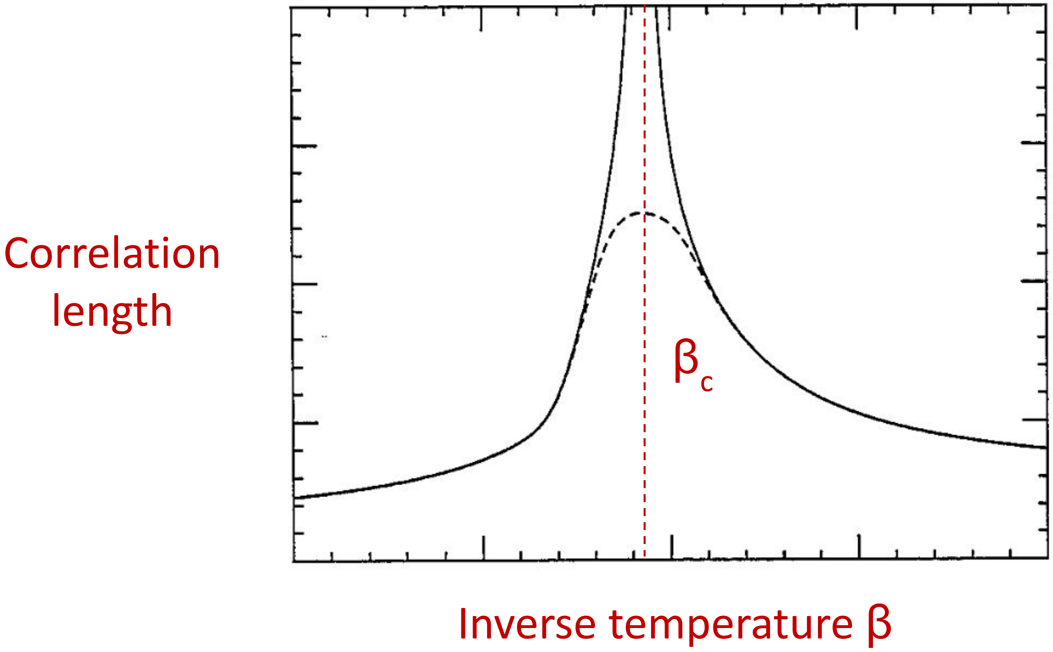
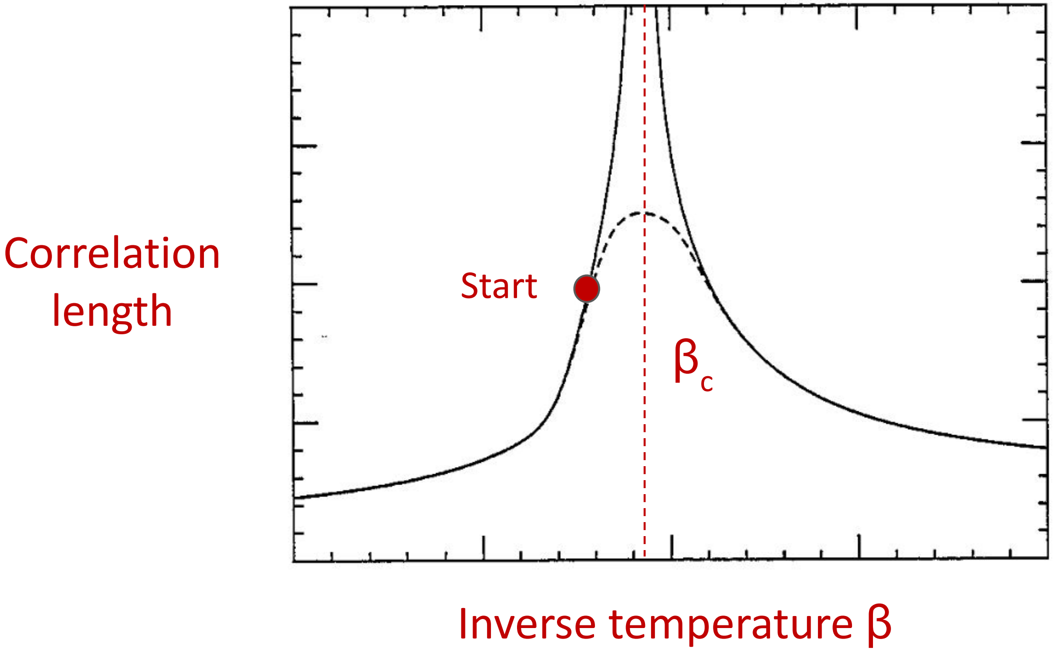


Altered figure from (Newman, Barkema) book (Fig 4.1)

Standard renormalization group



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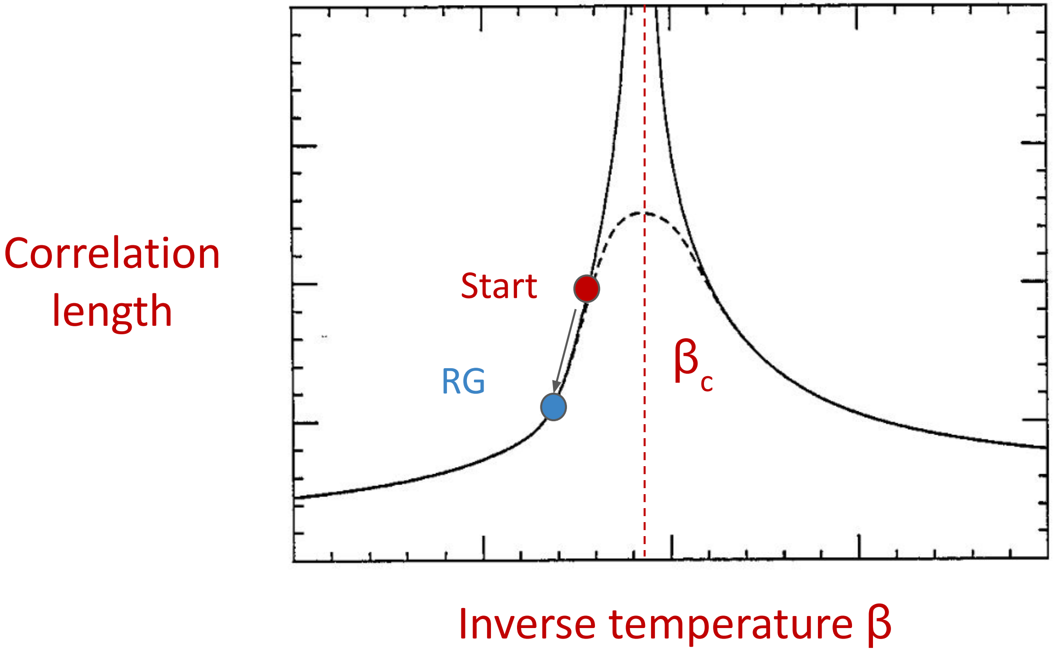

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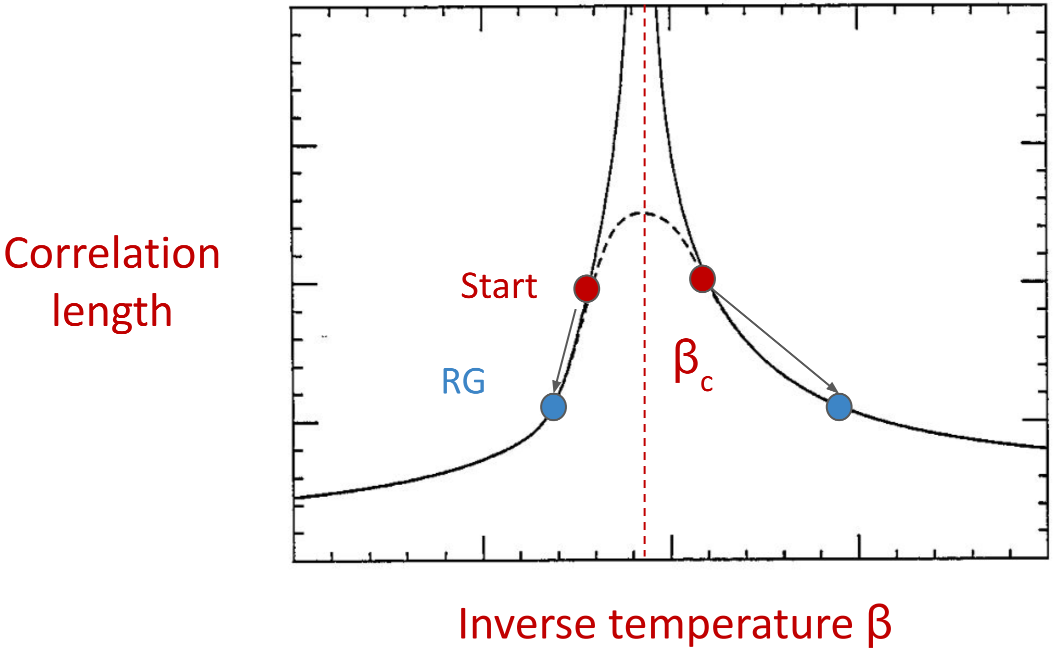

Altered figure from (Newman, Barkema) book (Fig 4.1)

Standard renormalization group

The Monte Carlo renormalization group (Swendsen, Phys. Rev. Lett. 42, 859, 1979) is a powerful technique to study phase transitions:

1) Each iteration of the MCRG (when done in the vicinity of the transition) drives the system closer to the fixed point: we reduce pertinent errors.
2) Calculations can be systematically improved via the consideration of multiple operators: the method performs superiorly to brute-force finite size scaling extrapolations.
3) We can partially eliminate finite-size effects: precision measurements can be obtained on smaller lattice volumes.
4) We can locate the critical point self-consistently: via the convergence of the critical exponents.
5) We linearize the transformation: we can obtain accurate results anywhere in the linear region (i.e. we do not need knowledge of the exact value of the critical point).
6) We need only one Monte Carlo simulation for a given lattice volume: we construct the renormalized configurations for other lattice volumes via the application of the real-space transformation.
7) There is no critical slowing down effect.

One limitation is that the standard MCRG can be applied for a finite number of steps before the degrees of freedom vanish.

Inverse renormalization group

Can we devise an inverse renormalization group approach that retains all of the benefits of the standard Monte Carlo renormalization group and can be applied, in principle, for an arbitrary number of times to iteratively increase the volume of the system?

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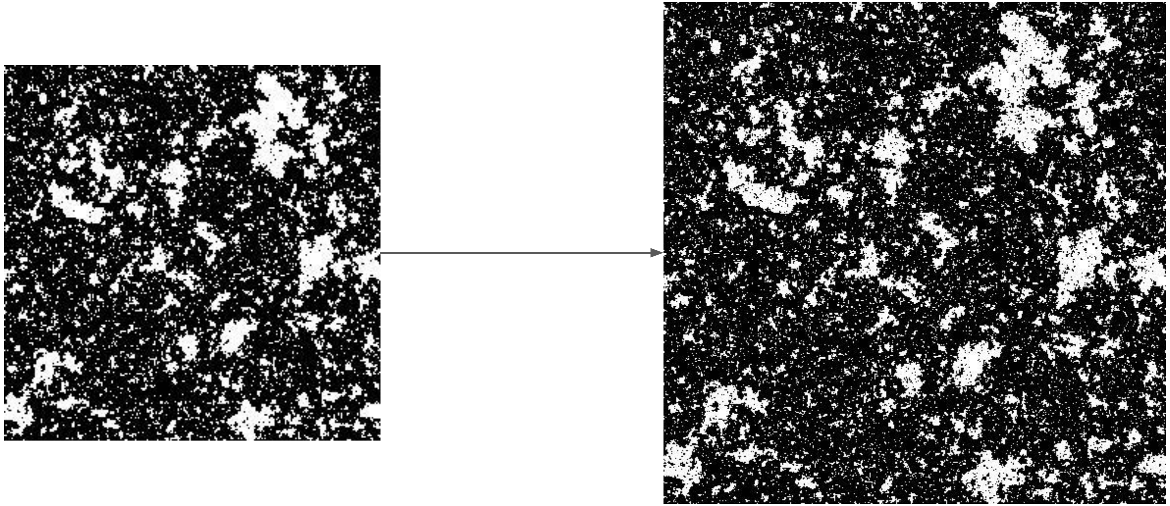
1. Inverse Monte Carlo Renormalization Group Transformations for Critical Phenomena, D. Ron, R. Swendsen, A. Brandt, Phys. Rev. Lett. 89, 275701, (2002).
2. Super-resolving the Ising model with convolutional neural networks, S. Efthymiou, MJS Beach, R. G. Melko, Phys. Rev. B 99, 075113, (2018).
3. Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603, (2022).
4. Inverse Renormalization Group of Disordered Systems, D. Bachtis, arXiv:2310.12631, (2023).

Inverse renormalization group

The first problem we encounter in the inverse renormalization group:

Novel degrees of freedom must be introduced within the system



Inverse renormalization group

Inversion of a majority rule in the **Ising** model

Original degree of freedom

+1

Possible rescaled degrees of freedom

+1	+1
+1	-1

-1	+1
+1	+1

-1	+1
+1	-1

-1	+1
+1	-1

…

Inverse renormalization group

Inversion of a summation in the $\boldsymbol{\varphi}^4$ model

Original degree of freedom

0.40

Possible rescaled degrees of freedom

0.01	0.36
0.02	0.01

-421.1	90.1
0.5	330.9

…

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

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Original degree of freedom

0.40

Possible rescaled degrees of freedom

0.01	0.36
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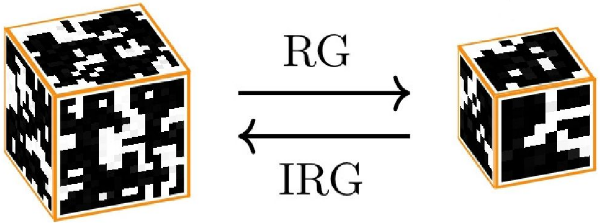
Too complicated!

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

<u>The main idea</u>:

We can learn a set of transformations, in the form of (transposed) convolutions, which approximate the inversion of a standard renormalization group transformation.



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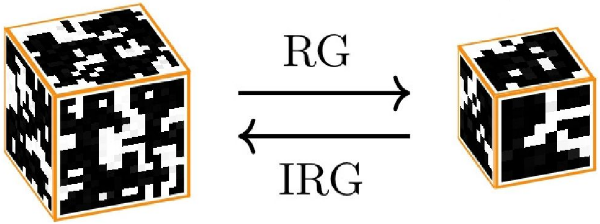


The benefit:

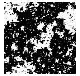
Convolutions can be applied irrespective of the lattice size: we can apply the inverse transformation an arbitrary number of times to construct configurations of increasing lattice size without the critical slowing down effect.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

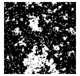
Inverse renormalization group

Why is there no critical slowing down effect in the inverse renormalization group?

L

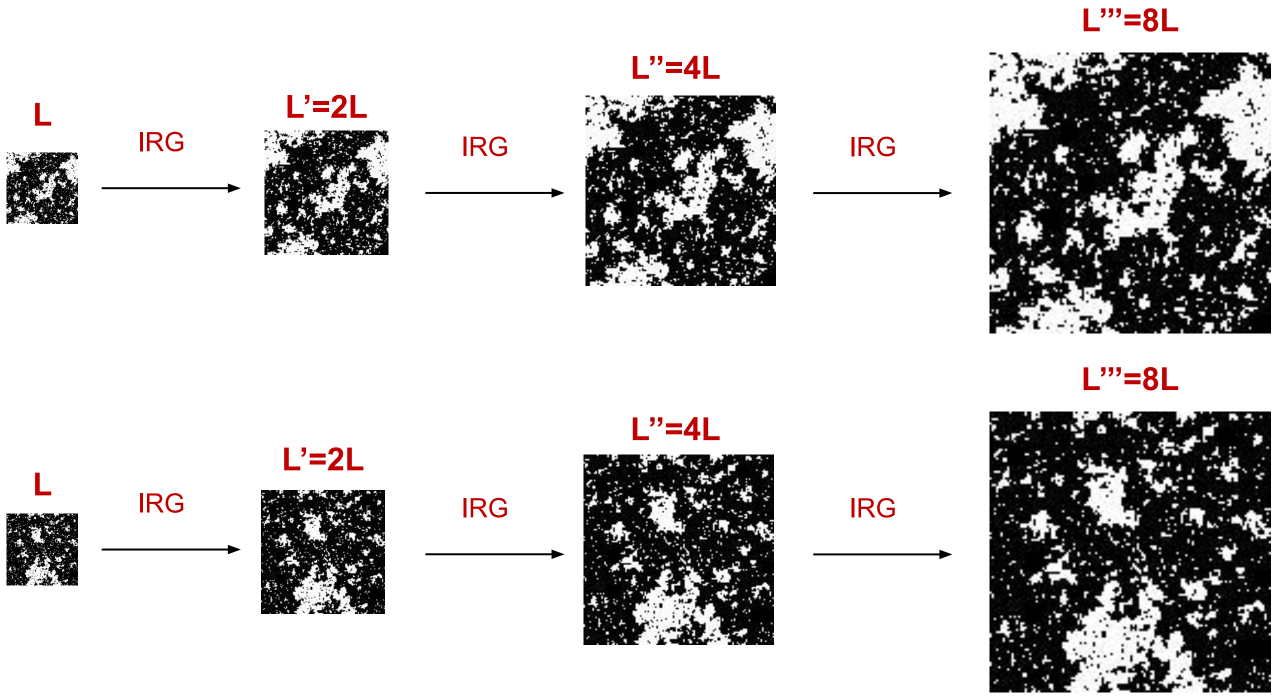


L



Inverse renormalization group

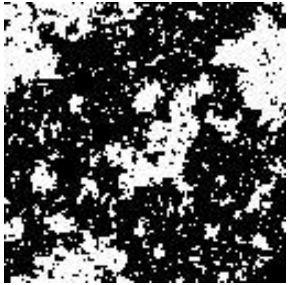
Why is there no critical slowing down effect in the inverse renormalization group?



Inverse renormalization group

Why is there no critical slowing down effect in the inverse renormalization group?

L'''=8L



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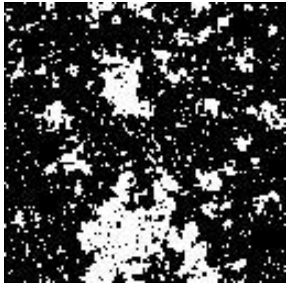
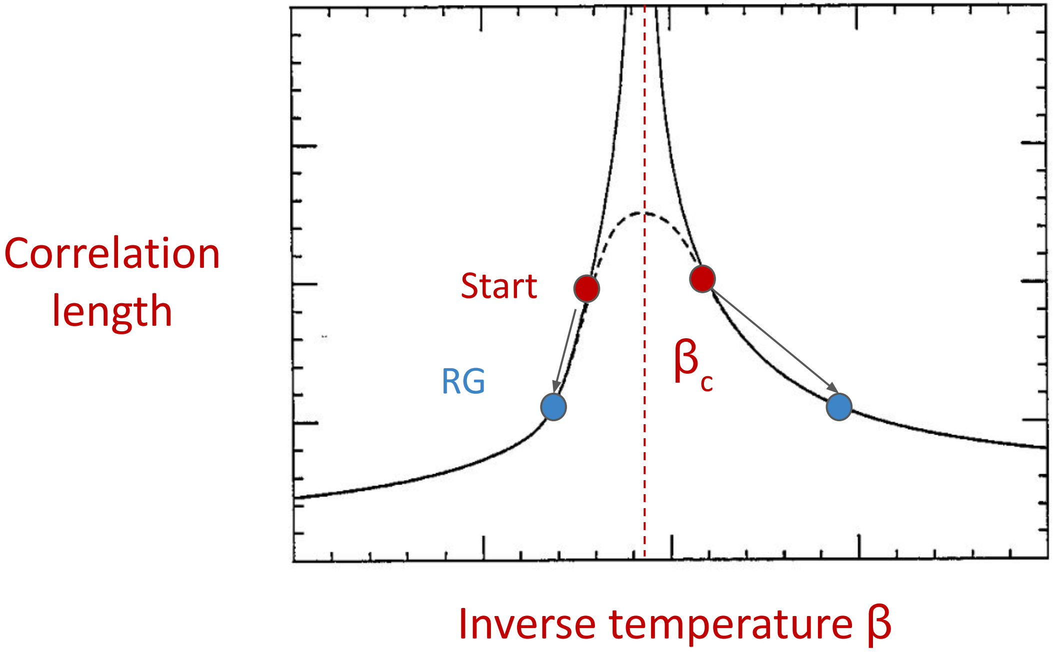


Standard renormalization group



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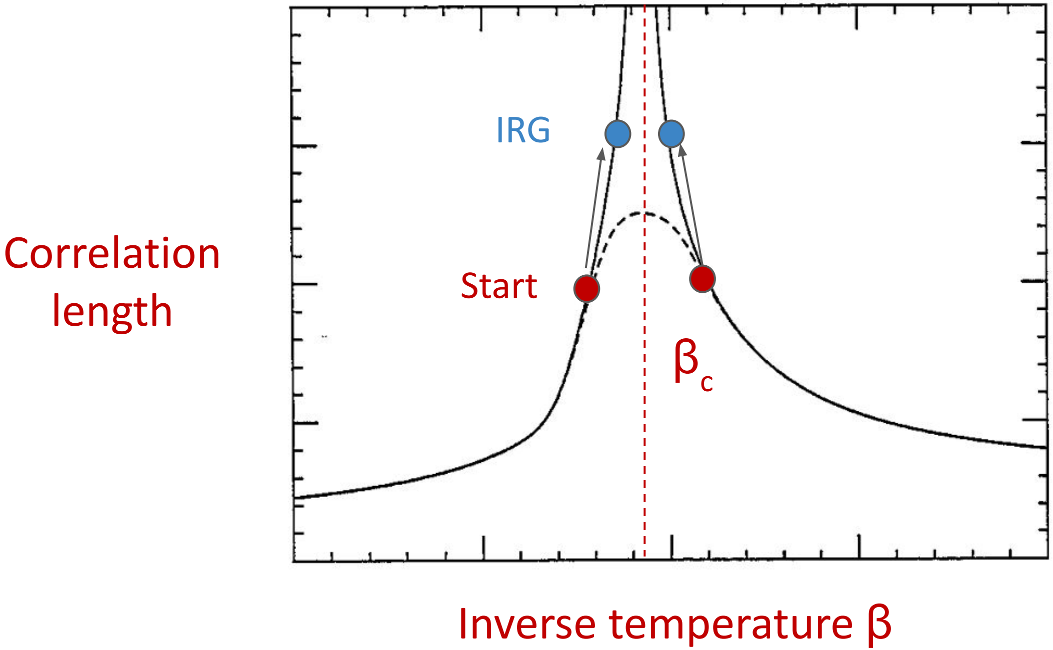

Inverse renormalization group

Certain steps to make the inverse renormalization group work efficiently
(2D φ^4 theory as an example):

1) Find a suitable standard renormalization group transformation for the system.
2) Verify that the standard renormalization group transformation is of high-quality (remember that the quality of the inverse transformation depends on the quality of the standard transformation)
3) Approximate the inversion of a standard renormalization group transformation with the use of machine learning techniques.
4) Start from a lattice size (L=32) and apply iteratively the inverse renormalization group to construct lattices of larger lattice volumes (up to L'=512).
5) Calculate quantities of interest.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Reducing finite-size effects with reweighted renormalization group transformations, D. Bachtis, Phys. Rev. E 109, 014125 (2024)

Inverse renormalization group

TABLE I. Values of the critical exponents γ/ν and β/ν. The original system has lattice size $L = 32$ in each dimension and its action has coupling constants $\mu_L^2 = -0.9515$, $\lambda_L = 0.7$, $\kappa_L = 1$. The rescaled systems are obtained through inverse renormalization group transformations.

L_i/L_j	32/64	32/128	32/256	32/512	64/128	64/256	64/512	128/256	128/512	256/512
γ/ν	1.735(5)	1.738(5)	1.741(5)	1.742(5)	1.742(5)	1.744(5)	1.744(5)	1.745(5)	1.745(5)	1.746(5)
β/ν	0.132(2)	0.130(2)	0.128(2)	0.128(2)	0.128(2)	0.127(2)	0.127(2)	0.126(2)	0.126(2)	0.126(2)

TABLE II. Values of the critical exponents γ/ν and β/ν. The original system has lattice size $L = 8$ in each dimension and its action has coupling constants $\mu_L^2 = -1.2723$, $\lambda_L = 1$, $\kappa_L = 1$. The rescaled systems are obtained through inverse renormalization group transformations.

L_i/L_j	8/16	8/32	8/64	8/128	8/256	8/512	16/32	16/64	16/128	16/256	16/512
γ/ν	1.694(6)	1.708(6)	1.717(6)	1.723(6)	1.727(6)	1.730(6)	1.721(6)	1.728(6)	1.732(6)	1.735(6)	1.737(6)
β/ν	0.154(2)	0.147(2)	0.142(2)	0.139(2)	0.137(2)	0.135(2)	0.140(2)	0.136(2)	0.134(2)	0.132(2)	0.131(2)

L_i/L_j	32/64	32/128	32/256	32/512	64/128	64/256	64/512	128/256	128/512	256/512
γ/ν	1.735(6)	1.738(6)	1.740(6)	1.740(6)	1.741(6)	1.742(6)	1.742(7)	1.743(6)	1.743(7)	1.743(7)
β/ν	0.133(2)	0.131(2)	0.130(2)	0.129(2)	0.129(2)	0.129(2)	0.128(2)	0.128(2)	0.127(2)	0.127(2)

Ising universality class: γ/ν=1.75, β/ν=0.125.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

The inverse renormalization group in disordered systems: 3D Edwards-Anderson spin glass

Inverse renormalization group

3D Edwards Anderson model

Paramagnetic phase
β->0

Spin Glass phase
β->∞

System freezes to a configuration

Replica theory

We consider two replicas σ,τ, of the system to define its two-replica Hamiltonian as:

$$E_{\sigma,\tau} = E_\sigma + E_\tau = -\sum_{\langle ij \rangle} J_{ij}(s_i s_j + t_i t_j),$$

where J_{ij} are random couplings drawn from a probability distribution.

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We can then define the overlap degrees of freedom $\rho_i = s_i t_i$, and we are able to calculate the overlap order parameter:

$$q_{\sigma\tau} = \frac{1}{V} \sum_i s_i t_i,$$

Inverse renormalization group

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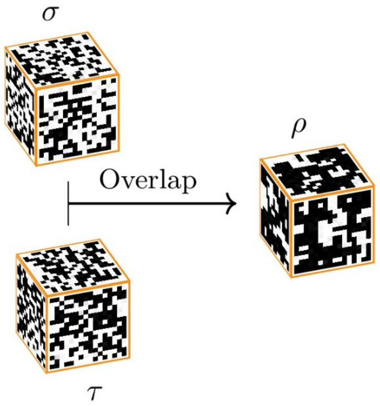
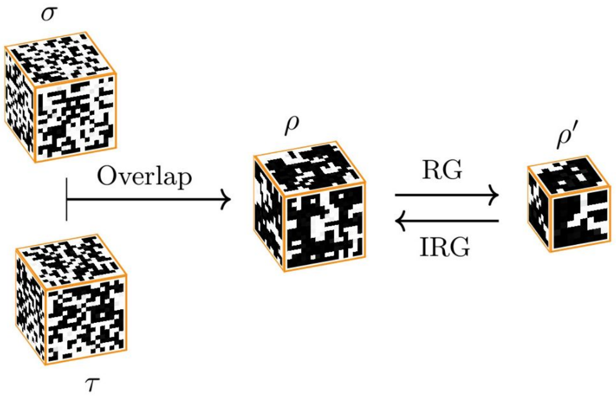


$$q_{\sigma\tau} = \frac{1}{V}\sum_i s_i t_i,$$

Inverse renormalization group

Overlap renormalization group

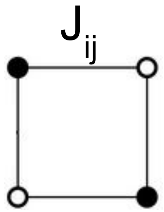


1) Relation of random and competing nonrandom couplings for spin-glasses, F. Haake, M. Lewenstein and M. Wilkens, Phys. Rev. Lett. 55 2606 (1985).
2) Monte Carlo renormalization-group study of Ising spin glasses, JS Wang and R. Swendsen, Phys. Rev. B 37 7745 (1988).
3) Overlap renormalization group transformations for disordered systems, D. Bachtis, Journal of Physics A: Mathematical and Theoretical (2024).

Inverse renormalization group

The 3D Edwards Anderson model is computationally hard:

$$E_{\sigma,\tau} = E_\sigma + E_\tau = -\sum_{\langle ij \rangle} J_{ij}(s_i s_j + t_i t_j),$$



Some problems:

1) $\{J_{ij}\}$ is drawn from a probability distribution.
2) We need replica exchange/parallel tempering techniques.
3) We need to simulate multiple replicas.

As an example: If we multiply all of the above L=8 requires approximately 160 million (independent) simulations.

Critical parameters of the three-dimensional Ising spin glass, Janus collaboration, Phys. Rev. B 88, 224416, 2013.

Inverse renormalization group

The largest lattice volume simulated for the 3D Edwards-Anderson model is

$V=40^3$

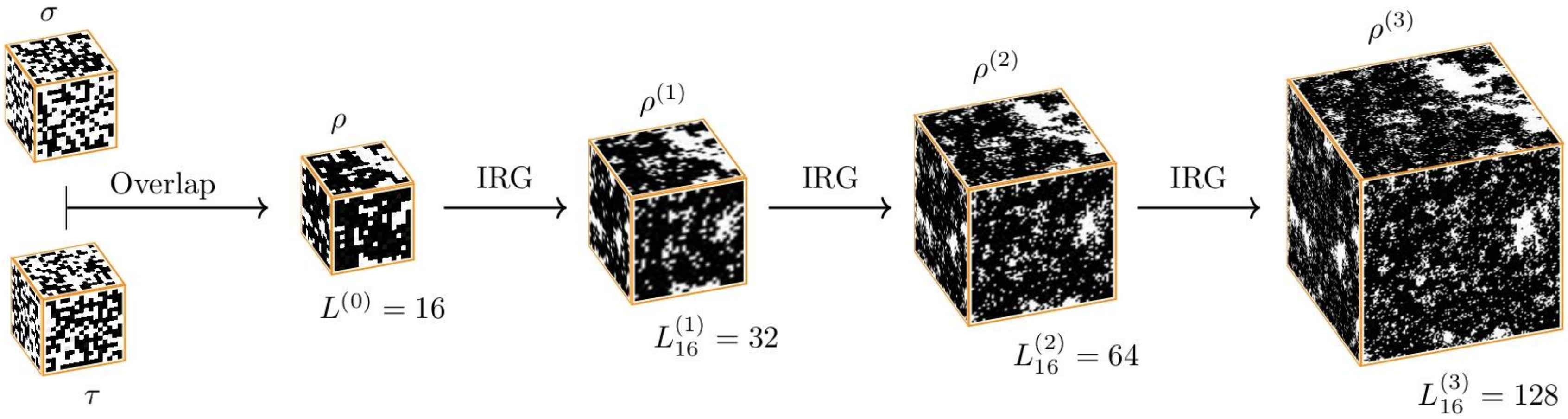
with the Janus dedicated supercomputer.

Critical parameters of the three-dimensional Ising spin glass, Janus collaboration, Phys. Rev. B 88, 224416, 2013.

Inverse renormalization group

Inverse renormalization group:

We are able to construct lattices up to V=128^3



Inverse Renormalization Group of Disordered Systems, D. Bachtis, arXiv:2310.12631, (2023).
Overlap renormalization group transformations for disordered systems, D. Bachtis, Journal of Physics A: Mathematical and Theoretical (2024).

Development of MCRG (obviously incomplete)

Monte Carlo renormalization group methods were first proposed Shang-keng Ma:

Renormalization Group by Monte Carlo Methods, Shang-keng Ma, Phys. Rev. Lett. 37, 461, (1976).

But the Monte Carlo renormalization group was turned into an efficient, competitive technique by Swendsen:

Monte Carlo Renormalization Group, RH Swendsen, Phys. Rev. Lett. 42, 859, (1979).

Wilson proposed a variation of MCRG methods:

Cargese Summer Institute: Recent Developments in Gauge Theories, K. Wilson, NATO Sci.Ser.B 59 (1980).

Series of developments

Monte Carlo Renormalization Group and Ising Models with n>~2, RH Swendsen and S. Krinsky, Phys. Rev. Lett. 43 (1979)

Optimization of Real-Space Renormalization-Group Transformations, RH Swendsen, Phys. Rev. Lett. 52, 2321 (1984)

Monte Carlo Calculation of Renormalized Coupling Parameters RH Swendsen, Phys. Rev. Lett. 52, 1165 (1984)

Gauge-Invariant Renormalization-Group Transformation without Gauge Fixing, RH. Swendsen, Phys. Rev. Lett. 47, 1775 (1981)

Monte Carlo Renormalization Group for SU(3) Lattice Gauge Theory, R. Gupta et al., Phys. Rev. Lett. 53, 1721 (1984)

Infrared Fixed Point of the 12-Fermion SU(3) Gauge Model Based on 2-Lattice Monte Carlo Renormalization-Group Matching, A. Hasenfratz, Phys. Rev. Lett. 108, 061601 (2012)

Development of inverse MCRG (obviously incomplete)

“Inverse” Monte Carlo renormalization group was attempted by:

Compagner, Hoogland, Blöte, (unpublished).

But the inverse Monte Carlo renormalization group was turned into an efficient, competitive technique by:

Inverse Monte Carlo Renormalization Group Transformations for Critical Phenomena, D. Ron, R. Swendsen, A. Brandt, Phys. Rev. Lett. 89, 275701 (2002)

Series of developments

Super-resolving the Ising model with convolutional neural networks, S. Efthymiou, MJS Beach, R. G. Melko, Phys. Rev. B 99, 075113, (2018).

Neural Network Renormalization Group, Shuo-Hui Li and Lei Wang, Phys. Rev. Lett. 121, 260601 (2018)

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, and B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Multiscale Data-Driven Energy Estimation and Generation, T. Marchand, M. Ozawa, G. Biroli, and S. Mallat, Phys. Rev. X 13, 041038 (2023) (see Misaki’s talk at this workshop)

Inverse Renormalization Group of Disordered Systems, D. Bachtis, arXiv:2310.12631, (2023).

Books

Chapter 9 of Binder-Landau, A Guide to Monte Carlo Simulations in Statistical Physics

Thank you for your attention!