Reinforcement Learning in Quantum Many-Body Physics and a Correspondence Between the Renormalization Group and Deep Neural Networks

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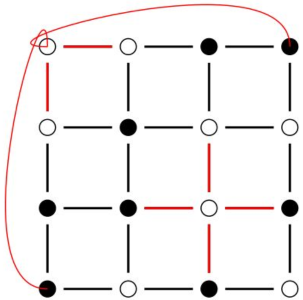
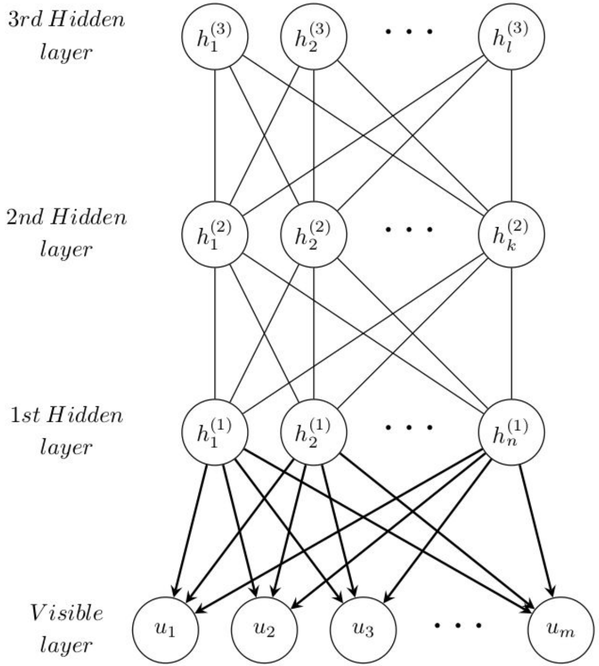
Overview

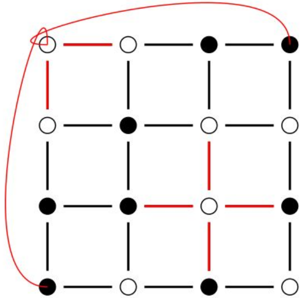
1. Unsupervised Learning of the Ising Model in d=2.
2. Studying Criticality with the Renormalization Group.
3. A Mapping Between Renormalization Group and Deep Neural Networks.
4. Reinforcement Learning in Many Body Physics.





The Ising Model in d=2

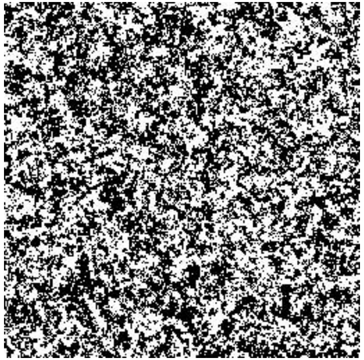
Hamiltonian: $$H = -\sum_{\langle ij \rangle} J_{ij} s_i s_j + B \sum_i s_i,$$



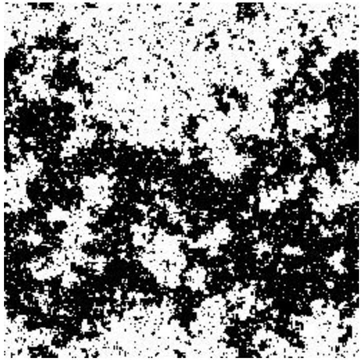
(Inverse) Temperature : β=1/T

Critical Temperature: $$\beta_c = \frac{1}{T_c} = \frac{1}{2}\ln(1+\sqrt{2}) \approx 0.44068679\ldots,$$

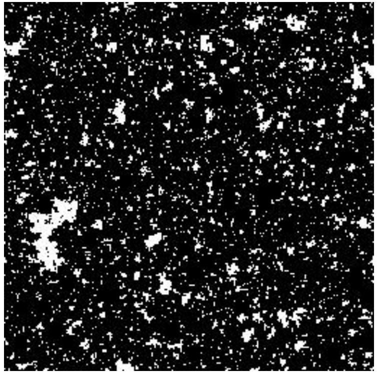
$\beta < \beta_c$



$\beta \cong \beta_c$



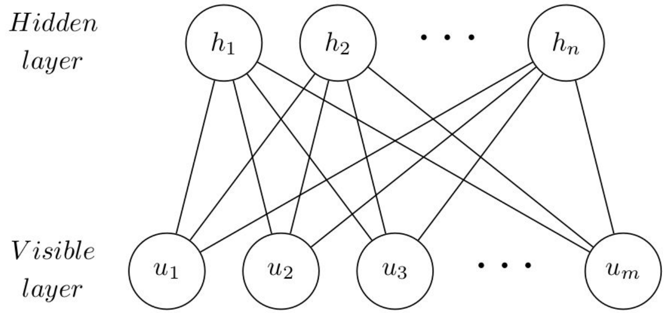
$\beta > \beta_c$



Restricted Boltzmann Machines

Energy function: $E(\boldsymbol{u}, \boldsymbol{h}) = -\sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij} h_i u_j - \sum_{j=1}^{m} b_j u_j - \sum_{i=1}^{n} c_i h_i$

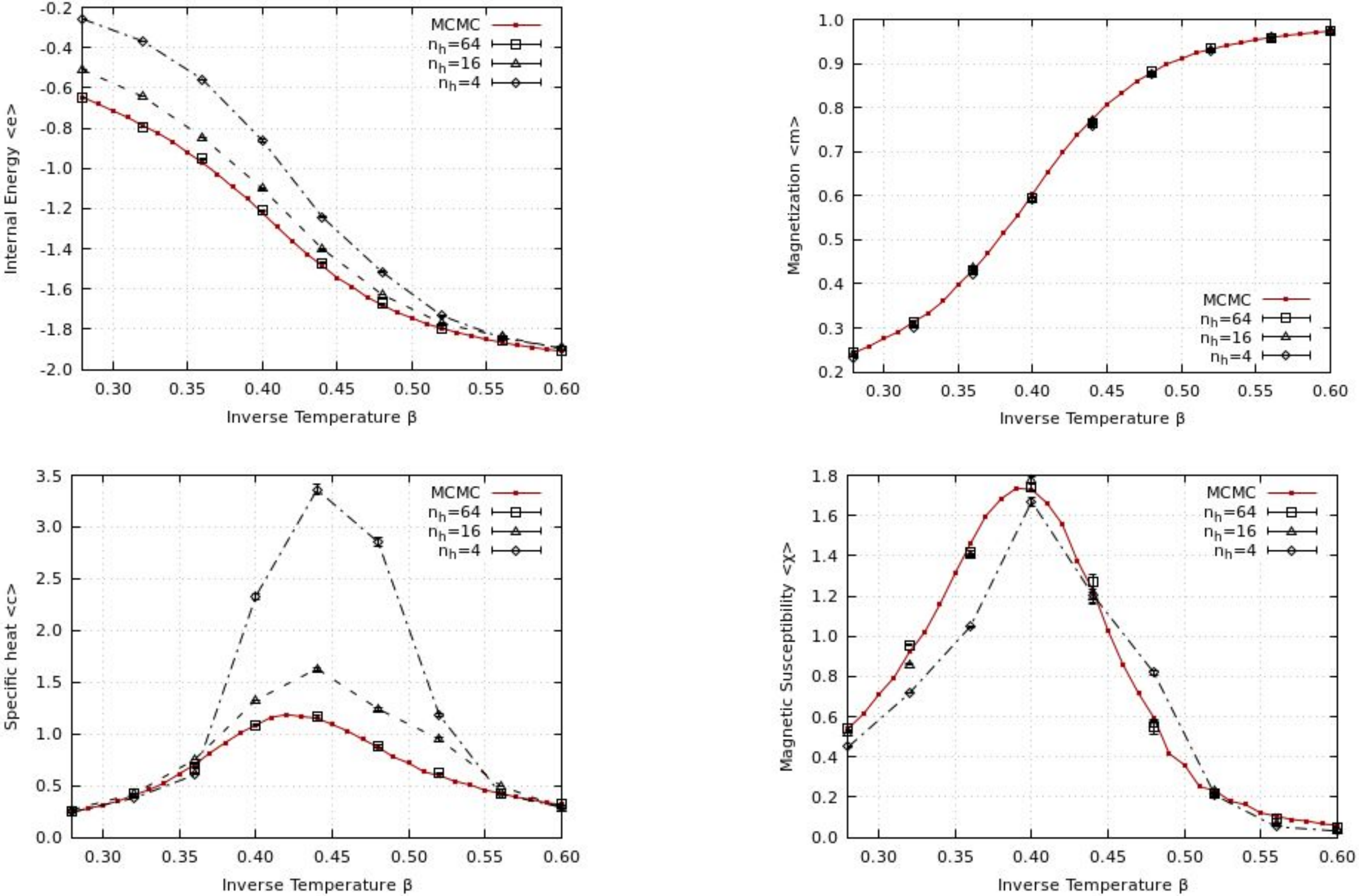
Joint probability distribution: $p(\boldsymbol{u}, \boldsymbol{h}) = \frac{1}{Z} e^{-E(\boldsymbol{u}, \boldsymbol{h})}$



- **Unsupervised Learning:**

Minimizing the **Kullback-Leibler Divergence:**

$$KL(q||p) = \sum_{\boldsymbol{x}\in\Omega} q(\boldsymbol{x}) \ln \frac{q(\boldsymbol{x})}{p(\boldsymbol{x})} = \sum_{\boldsymbol{x}\in\Omega} q(\boldsymbol{x}) \ln q(\boldsymbol{x}) - \sum_{\boldsymbol{x}\in\Omega} q(\boldsymbol{x}) \ln p(\boldsymbol{x})$$

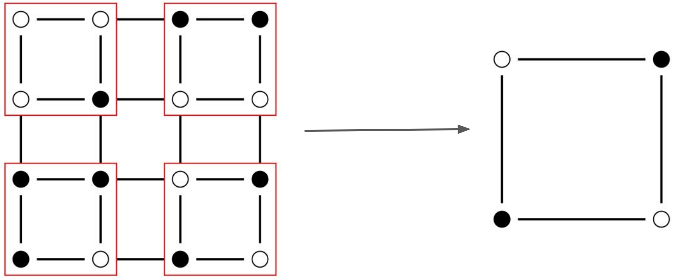


Internal Energy <e>
Inverse Temperature β
MCMC
n_h=64
n_h=16
n_h=4
Magnetization <m>
Specific heat <c>
Magnetic Susceptibility <χ>

The Real-Space Renormalization Group

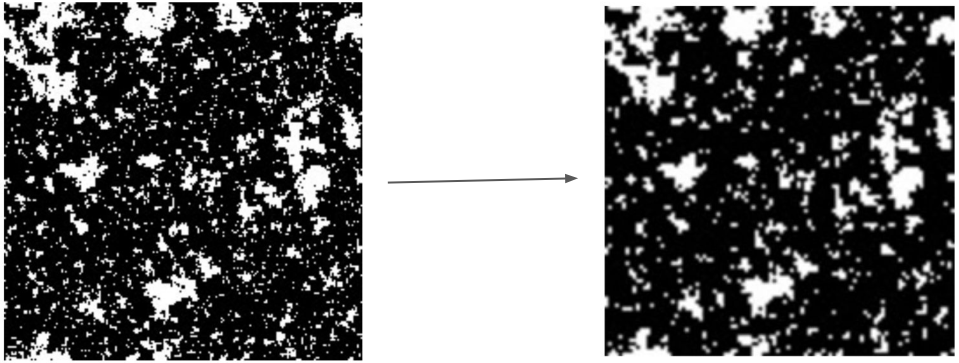
Rescaling Factor **b**: $L' = \frac{L}{b}$

The method introduces **uncontrolled** errors.



Original System N=200*200

Rescaled System N=100*100



The Real-Space Renormalization Group

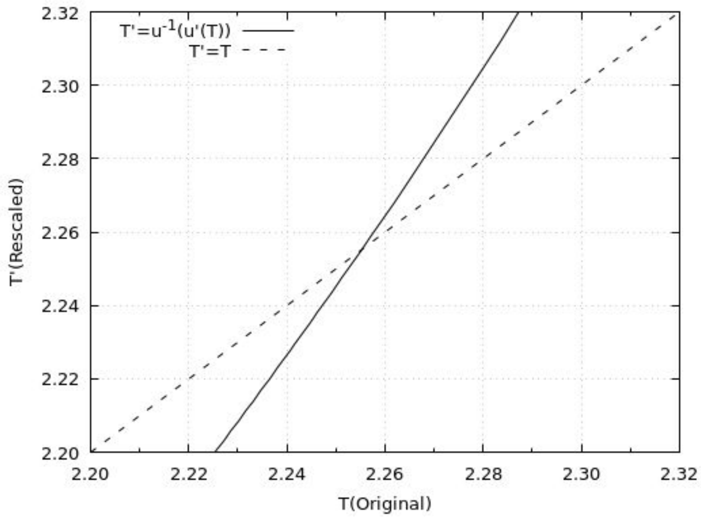
Rescaled Correlation Length: $\xi' = \frac{\xi}{b}$

At **critical temperature** both systems have the **same** correlation length **and** the **same** intensive quantities:

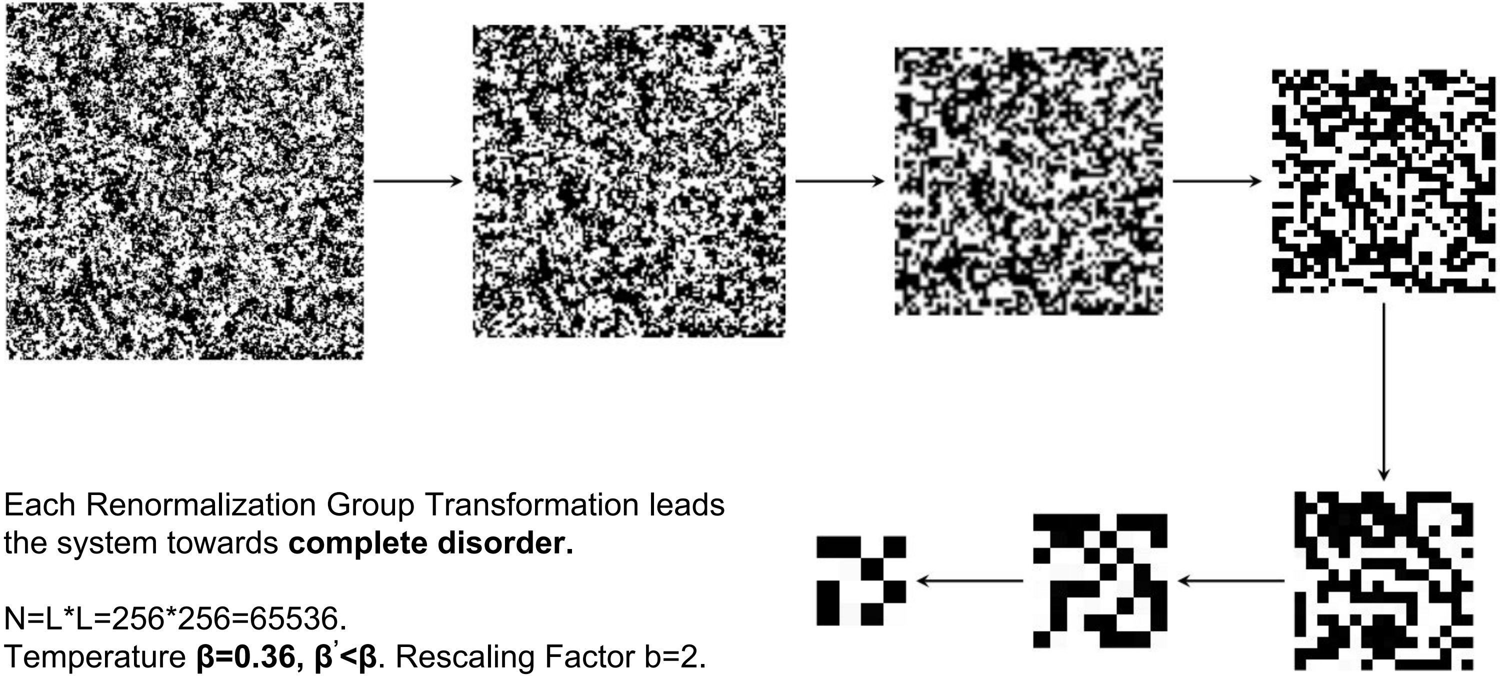
$$\xi = \xi' \quad , \quad u'(T) = u(T')$$

Mapping: $T' = u^{-1}(u'(T))$

Critical Fixed Point: T_c=2.269...



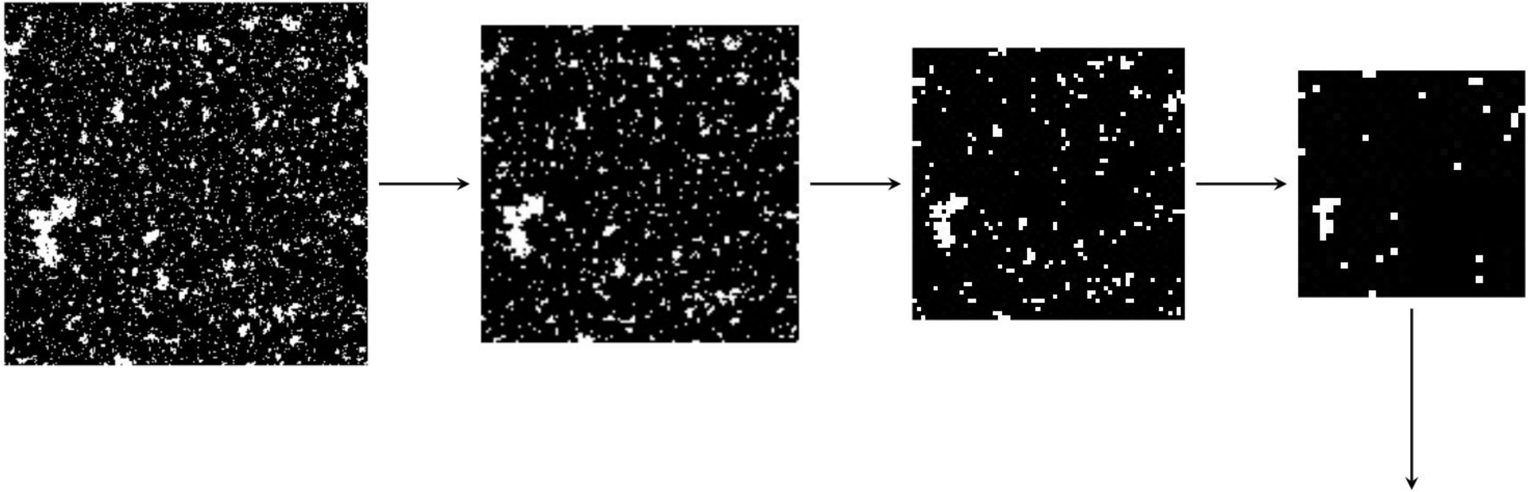
The Real-Space Renormalization Group

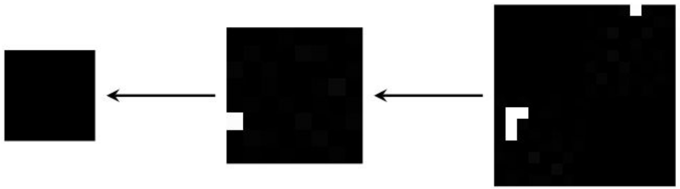


Each Renormalization Group Transformation leads the system towards **complete disorder.**

N=L*L=256*256=65536.
Temperature **β=0.36, β'<β**. Rescaling Factor b=2.

The Real-Space Renormalization Group

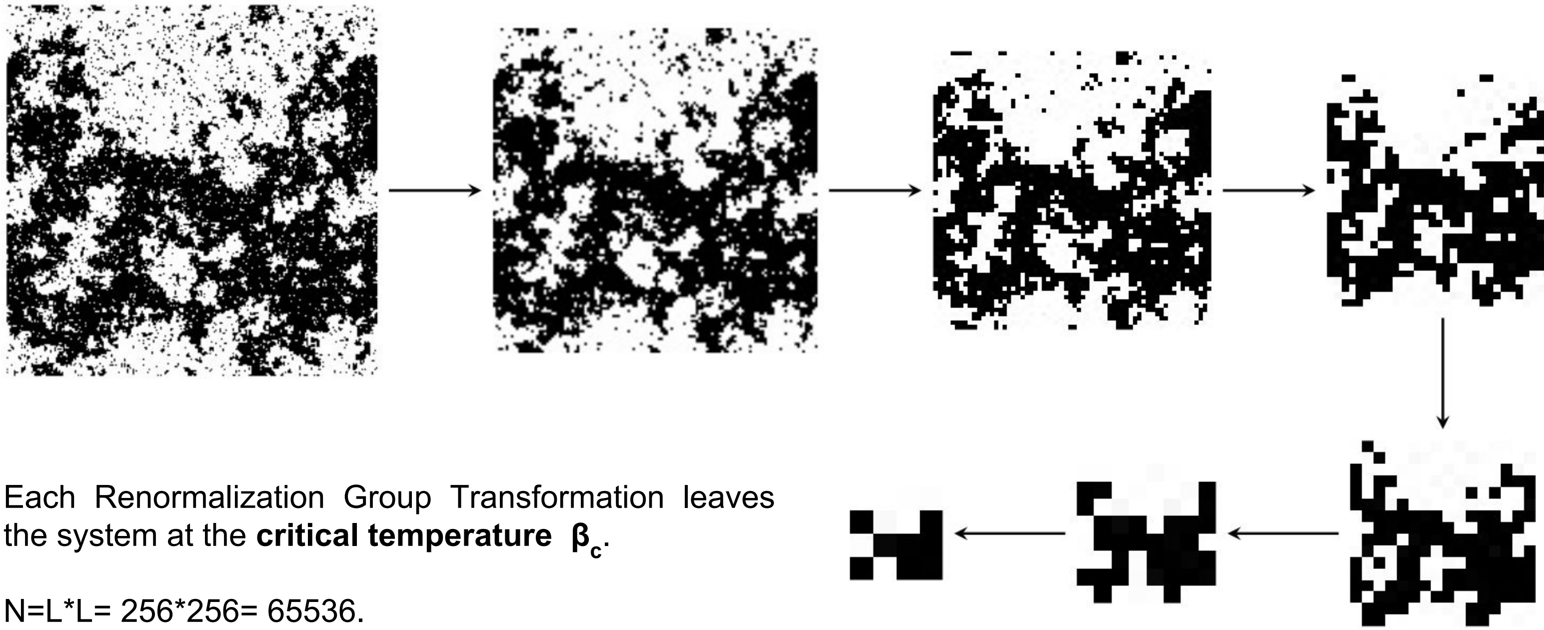




Each Renormalization Group Transformation leads the system towards **complete order**.

N=L*L=256*256=65536.
Temperature **β=0.45, β'>β**. Rescaling Factor b=2.

The Real-Space Renormalization Group



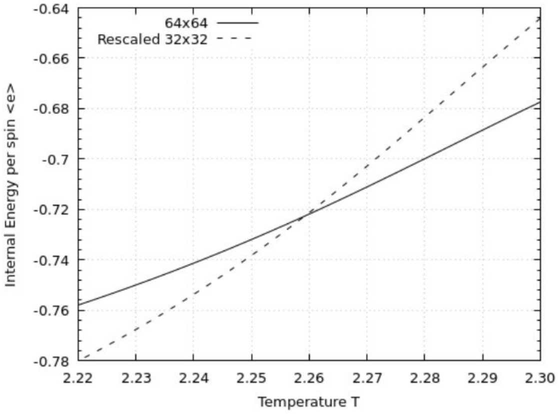
Each Renormalization Group Transformation leaves the system at the **critical temperature β_c**.

N=L*L= 256*256= 65536.
Temperature **$\beta_c \cong$ 0.4407, β'**= **β_c**. Rescaling Factor b=2.

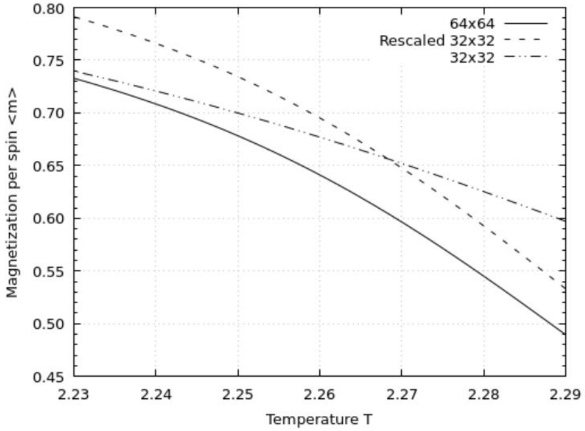
The Real-Space Renormalization Group

(Some) Critical Exponents:

$$correlation\,length\,\xi \sim |t|^{-\nu}$$
$$specific\,heat\,C \sim |t|^{-a}$$
$$magnetization\,M \sim |t|^{\beta}$$
$$magnetic\,susceptibility\,\chi \sim |t|^{\gamma}$$



Onsager's Exponents: $\nu = 1,\ a = 0,\ \beta = \frac{1}{8},\ \gamma = \frac{7}{4}$



Estimations : ν ≅ 1.01, α ≅ -0.19, β ≅ 0.101, γ ≅ 1.744

The Renormalization Group and Deep Belief Networks

Original System: $H[\{u_i\}] = -\sum_i K_i u_i - \sum_{i,j} K_{ij} u_i u_j - \sum_{i,j,k} K_{ijk} u_i u_j u_k + \dots$

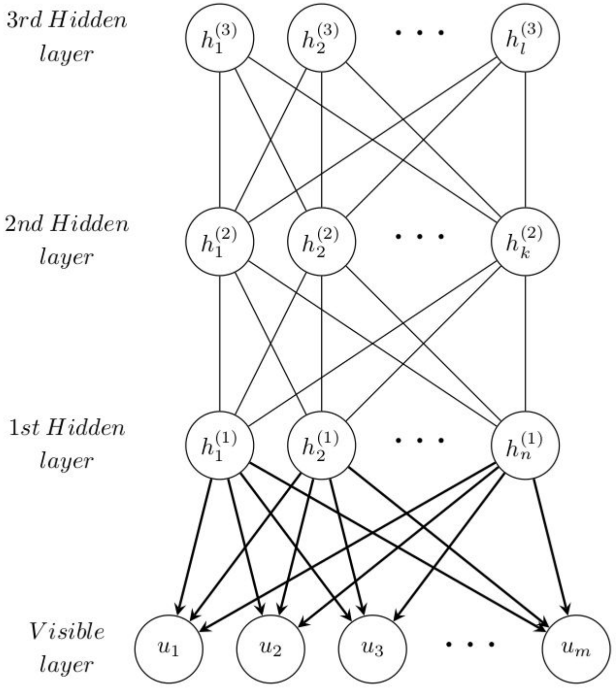
Rescaled System: $H^{RG}(\{h_j\}) = -\sum_i K_i^{'} h_i - \sum_{i,j} K_{ij}^{'} h_i h_j - \sum_{i,j,k} K_{ijk}^{'} h_i h_j h_k + \dots$

Variational Operator: $T(\{u_i\}, \{h_j\}) = -E(\{u_i\}, \{h_j\}) + H[\{u_i\}]$

For an exact transformation:

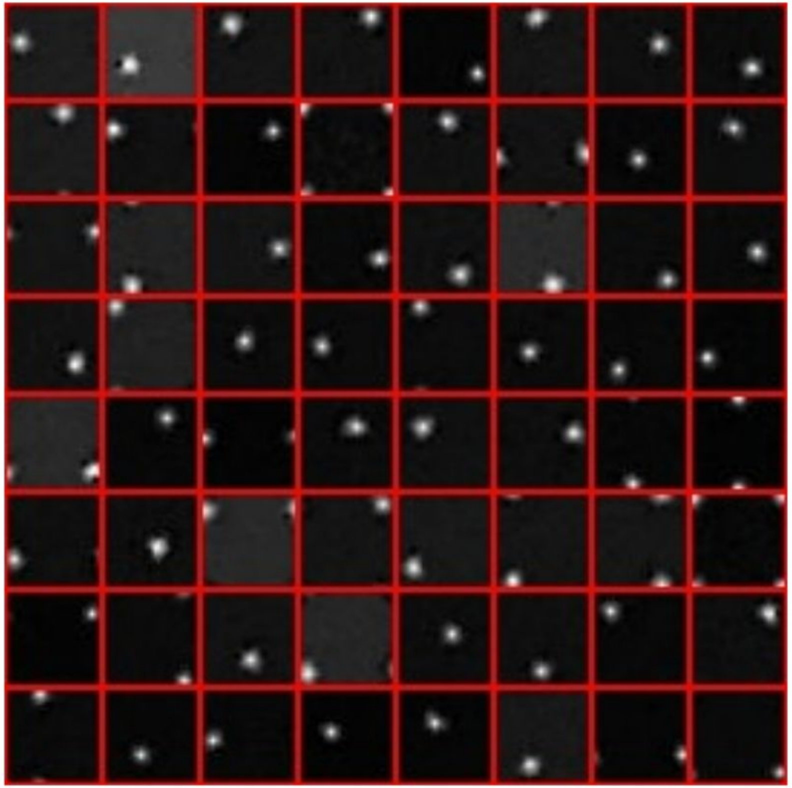
$$H_\lambda^{RG}[\{h_j\}] = H_\lambda^{RBM}[\{h_j\}]$$

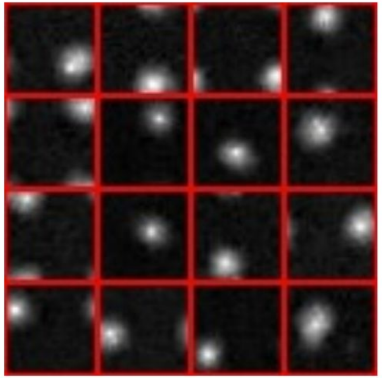
$$H[\{u_i\}] = H_\lambda^{RBM}[\{u_i\}]$$



m=1024, n=256, k=64, l=16

The Renormalization Group and Deep Belief Networks



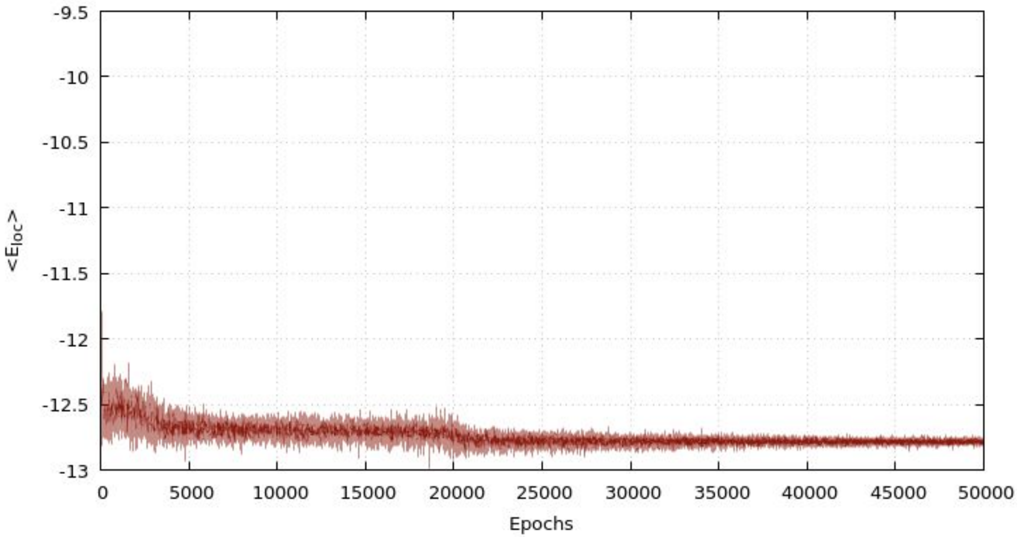


Reinforcement Learning: The Transverse-field Ising Model in d=1

Variational Principle: $$E_{gs} \leq \langle H \rangle_{var} = \frac{\langle \psi_{var} | H | \psi_{var} \rangle}{\langle \psi_{var} | \psi_{var} \rangle} \equiv \mathcal{F}[\psi_{var}]$$

Variational Monte Carlo: $$\langle \mathcal{O} \rangle = \frac{\sum_x |\psi_{var}(x)|^2 \mathcal{O}_{loc}}{\sum_x |\psi_{var}(x)|^2}$$

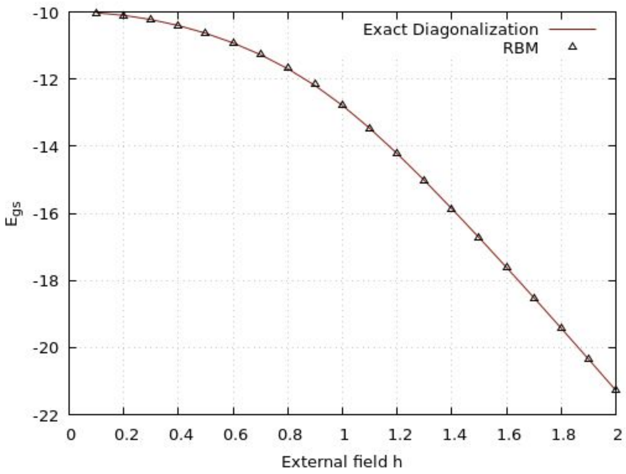
RBM Training for h=1.0

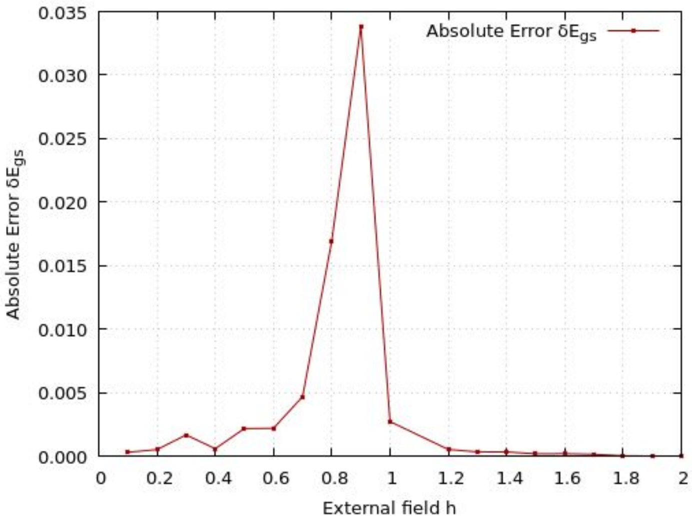


Neural Network Quantum States:

$$\Psi(\sigma_1^z, \sigma_2^z, \dots \sigma_N^z) = \sqrt{F_{rbm}(\sigma_1^z, \sigma_2^z, \dots \sigma_N^z)}$$

Reinforcement Learning: The Transverse-field Ising Model in d=1





Summary

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D. Reinforcement Learning in Many Body Physics.

Thank you for your attention!