Università di Pisa

Monte Carlo simulation of the Ising model

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Ising Model

Hamiltonian

$$H = -J \sum_{<ij>} s_i s_j - h \sum_i s_i$$

$$J = 1,\ h = 0$$

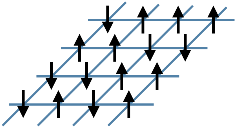
Order parameter

Spontaneous breaking of $\mathbb{Z}_2$ symmetry, if $N \to \infty$

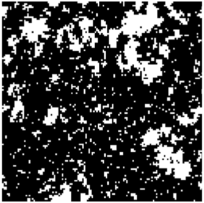
$$m = \langle s_i \rangle$$

For finite N it would always be m=0, so I instead take

$$m = \lim_{N\to\infty} \frac{1}{N} \left\langle \left| \sum_i s_i \right| \right\rangle$$



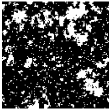
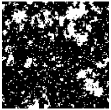
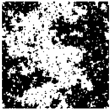
2D lattice with spin s_i. Up and down arrows correspond to values +1 or -1.



Plot of a square lattice, L=128, N=L^2.

Monte Carlo

Simulating interaction with a **thermal bath**.

 $\Rightarrow$  $\Rightarrow \dots \Rightarrow$ 

μ ν ω

Metropolis algorithm

- Choose a uniform probability ($\frac{1}{N}$) of a spin to be flipped;
- Accept to be flipped with a probability

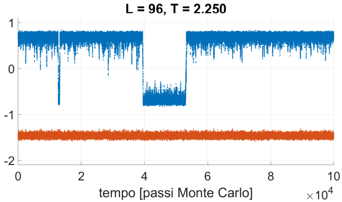
$$A(\mu \to \nu) = \begin{cases} 1 & \text{se } E_\nu < E_\mu \\ e^{-(E_\nu - E_\mu)/k_B T} & \text{se } E_\nu > E_\mu \end{cases} .$$

(μ starting state, ν state with spin flipped)

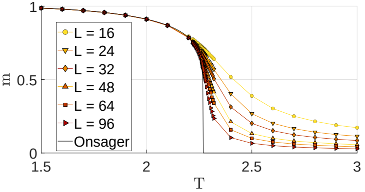
Guarantees **ergodicity** and **detailed balance**.

Numerical simulations

Run the algorithm for different temperatures T and different lattice sizes L.



Average magnetization and energy per spin, measured at every Monte Carlo time step.

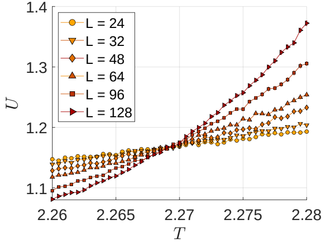


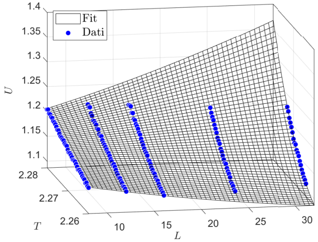
Average magnetization as a function of temperature, for different lattice sizes.

Resulting data is correlated

Use bootstrap with blocking to estimate the error.

Scaling and universality





Second order phase transitions

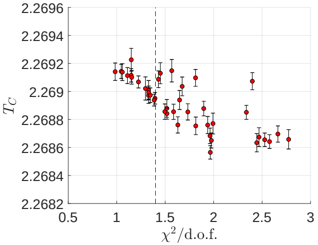
- Thermodynamical quantities have **exponential behavior** near the critical temperature;
- The **critical exponents** do not depend on the microscopic details of the system.

Binder cumulant $U = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$

Close to T_c has the form

$$U(T, L) = f\left((T - T_c)L^{1/\nu}\right)$$

Fit results



	Expected	Estimated
T_c	2.2692...	2.2691(2)
ν	1	1.01(5)
U^*	1.168...	1.167(2)
β	0.125	0.124(8)
γ	1.75	1.75(10)
α	0	0.0(6)

Fit with different hypotesis $\rightarrow$ estimate of **systematic errors**

Where do they come from?

- ignored the corrections to scaling ($\sim L^{-\omega}$)
- expanded f only to first order
- choice of values range
- ...

Other exponents

$$m(T) = L^{-\beta/\nu} f\left((T - T_c)L^{1/\nu}\right)$$

Thank you.

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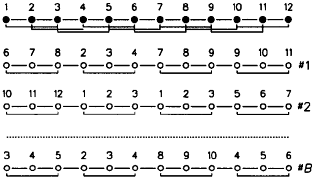
Appendix 1: Moving block bootstrap



Example: $n = 12$, $m = 3$, $k = 4$.

- Array of length n
- Divided in all possible blocks of length m
- Sample k blocks with repetitions, with $n \simeq k \times l$
- Repeat B times

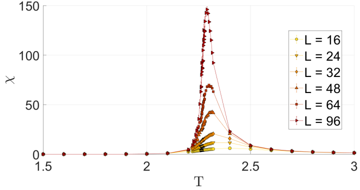
Call θ_b the average of every array, with $b = 1, ..., B$.

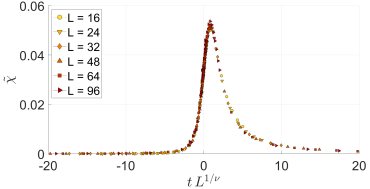
Error estimate

$$\sigma(\theta) = \sqrt{\sum_{b=1}^{B} \frac{(\theta_b - \overline{\theta}\,)^2}{B-1}}, \qquad \overline{\theta} = \frac{1}{B} \sum_{b=1}^{B} \theta_b$$

Mignani, S Rosa, R 1995, “The moving block bootstrap to assess the accuracy of statistical estimates in Ising model simulations”, Computer Physics Communications 92, 203-213.

Appendix 2: Finite Size Scaling





Average magnetic susceptibility

$$\chi = \frac{N}{k_B T}\left(\langle m^2 \rangle - \langle m \rangle^2\right)$$

Correlation length ξ

$$G_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \sim e^{-|i-j|/\xi}$$

Call $t = \frac{T-T_c}{T_c}$

In the thermodynamical limit $\xi \sim |t|^{-\nu},\ \chi \sim |t|^{-\gamma} \ \Rightarrow\ \chi \sim \xi^{\gamma/\nu}$

So for finite L $\ \xi \xrightarrow[t\to 0]{} L$: $\ \chi = \xi^{\gamma/\nu}\chi_0(L/\xi)$

Define $\ \tilde{\chi}(x^{1/\nu})\, x^{\gamma} = \chi_0(x)$ to get rid of ξ

$$\chi(L,T) = L^{\gamma/\nu}\tilde{\chi}(L^{1/\nu}|t|)$$