Critical behavior and scaling

Correlation length ξ defined in terms of correlation function $C(\vec{r}_{ij}) = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle^2 \sim e^{-r_{ij}/\xi}, \quad \vec{r}_{ij} \equiv |\vec{r}_i - \vec{r}_j|$

The correlation length diverges at the critical point

$$\xi \sim t^{-\nu}, \quad t = \frac{|T - T_c|}{T_c}$$
 (reduced temperature)

v is an example of a critical exponent

Universality

Critical exponents do not depend on microscopic details of the interactions; only on the dimensionality of the system and the order parameter:

- Ising, gas/liquid (scalar Z2-symmetric order parameter)
- XY spins, phase of superconductor (2D, O(2) order parameter)
- Heisenberg spins (3D, O(3) order parameter) Phase transitions fall into universality classes characterized by different sets of critical exponents

Other critical exponents

Order parameter for T < Tc (e.g., magnetization)

 $\langle m \rangle \sim (T_c - T)^{\beta}$

In practice, calculate $\langle |m| \rangle$, $\langle m^2 \rangle$ Susceptibility corresponding to order

$$\chi = \frac{1}{N} \frac{1}{T} \left(\langle M^2 \rangle - \langle |M| \rangle^2 \right)$$

Diverges at the critical point

$$\chi \sim t^{-\gamma}$$

Specific heat $C = \frac{1}{N} \frac{1}{T^2} (\langle E^2 \rangle - \langle E \rangle^2)$

Singular at Tc

$$C \sim t^{-\alpha}$$

The exponent α can be positive or negative (no divergence If negative; 0 can correspond to log divergence)



Magnetization of 2D Ising ferromagnet

 $\langle |m| \rangle \sim (T_c - T)^{\beta}, \quad (T < T_c)$ for infinite system



Magnetization squared $\langle m^2 \rangle \sim (T_c - T)^{2\beta}$, $(T < T_c)$



The exponent β can be extracted for large L

Comparison with known 2D Ising model exponent $\beta=1/8$



If Tc is not known, use it as an adjustable parameter and look for power-law behavior

Finite-size scaling

For a system of length L, the correlation length $\xi \leq L$ Express divergent quantities in terms of correlation length, e.g.,

$$\xi \sim t^{-\nu}, \quad \chi \sim t^{-\gamma} \sim \xi^{\gamma/\nu}$$

The largest value is obtained by substituting $\xi \to L$ $\chi_{\rm max} \sim L^{\gamma/\nu}$

At what T does the maximum occur?

 $\xi = at^{-\nu} = L \implies t \sim L^{-1/\nu}$

The peak position of a divergent quantity can be taken as Tc for finite L (different quantities will give different Tc) γ, ν can be extracted by studying peaks in $\xi(T)$

Similarly for specific heat;

 $C_{\rm max} \sim L^{\alpha/\nu}$

Susceptibility:
$$\chi = \frac{1}{N} \frac{1}{T} \left(\langle M^2 \rangle - \langle |M| \rangle^2 \right)$$



Diverges at the transition: $\chi \sim |T - T_c|^{-\gamma}$

On a logarithmic scale



Specific heat



 $C \sim |T - T_c|^{-\alpha}$

(actually $\alpha=0$ and log divergence for 2D Ising)

2D Ising model; $\gamma = 7/4$, $\nu = 1$ $T_c = 2/\ln(1 + \sqrt{2}) \approx 2.2692$



In general; find Tc and exponents so that large-L curves scale

Binder ratio $Q = \frac{\langle m^2 \rangle}{\langle |m| \rangle^2} \qquad \left(Q_{2n} = \frac{\langle m^{2n} \rangle}{\langle m^n \rangle^2}, \quad n = 1, 2, \ldots \right)$

Useful dimensionless quantity for accurately locating Tc Infinite-size behavior:

$$\langle |m| \rangle \sim t^{\beta}$$

$$\langle m^2 \rangle \sim t^{2\beta}$$

Implies finite-size scaling forms

 $\langle m^2 \rangle \sim L^{-2\beta/\nu}$

$$\langle |m| \rangle \sim L^{-\beta/\nu}$$

Hence Q should be size-independent at the critical point

 $Q \to 1 \text{ for } T \to 0, \quad Q \to \text{ constant for } T \to \infty$

Q(L) curves for different L cross at Tc; often small corrections



Q is size independent at Tc (useful for locating Tc)



Scaling theory with corrections predicts: $T^*(L, 2L) = T_c + aL^{-(1/\nu+\omega)}$

 ω is an exponent governing scaling corrections, $\omega=2$ for 2D Ising

Crossing points for, e.g., sizes L, 2L can be extrapolated to infinite L to give an accurate value for Tc



Autocorrelation functions

Value of some quantity at Monte Carlo step i: Q_i

The autocorrelation function measures how a quantity becomes statistically independent from its value at previous steps

$$A_Q(\tau) = \frac{\langle Q_{i+\tau}Q_i \rangle - \langle Q_i \rangle^2}{\langle Q_i^2 \rangle - \langle Q_i \rangle^2} \quad \text{(averaged over time i)}$$

Asymptotical decay

 $A_Q(\tau) \sim e^{-\tau/\Theta}, \quad \Theta =$ autocorrelation time

Integerated autocorrelation time

$$\Theta_{\rm int} = \frac{1}{2} + \sum_{\tau=1}^{\infty} A_Q(\tau)$$

Critical slowing down

 $\Theta \to \infty$ as $T \to T_c$

At a critical point for system of length L; Q=order parameter

 $\Theta \sim L^z$, z = dynamic exponent

General finite-size scaling hypothesis

The ratio $\xi/L = t^{-\nu}L^{-1}$ should control the behavior of finite-size data also close to Tc

Test this finite-size scaling form

 $\chi(t) = L^{\sigma} f(\xi/L) = L^{\sigma} f(t^{-\nu} L^{-1}) = L^{\sigma} g(t L^{1/\nu})$

What is the exponent σ ?

We know that for fixed (small) t, the infinite L form should be (i)

 $\chi(t) \sim t^{-\gamma}, \quad (L \to \infty)$

To reproduce this, the scaling function g(x) must have the limit

 $g(x) \to x^b, \quad (x \to \infty)$

We can determine the exponents as follows

 $\chi(t) \sim L^{\sigma}g(tL^{1/\nu}) = L^{\sigma}(tL^{1/\nu})^b = t^bL^{\sigma+b/\nu}$

Hence $b = -\gamma, \ \sigma = \gamma/\nu$

 $\chi(t) = L^{\gamma/\nu} g(t L^{1/\nu})$

Find g by graphing $\chi(t)/L^{\gamma/\nu}$ versus $tL^{1/\nu}$

2D Ising autocorrelation functions for IMI



Exponentially decaying autocorrelation function - convergent autocorrelation time as L increases



Autocorrelation time diverges with L

Critical slowing down Dynamic exponent Z: $\Theta, \Theta_{int} \sim L^Z$



For the Metropolis algorithm (Metropolis dynamics) $Z \approx 2.2$

How to calculate autocorrelation functions

If we want autocorrelations for up to K MC step separations, we need to store K successive measurements of quantity Q Store values in vector tobs[1:K]; first k steps to fill the vector. Then, shift values after each step, add latest measurement:

```
vector contents after MC step n
```



Accumulate time-averaged correlation functions of Q (variable q)

```
for t=2:k
   tobs[t]=tobs[t-1]
end
tobs[1]=q
for t=0:k-1
   acorr[t]=acorr[t]+tobs[1]*tobs[1+t]
end
```