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 $\xi \rightarrow L$

$$\chi_{\text{max}} \sim L^{\gamma/\nu}$$

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 $T_c$ for finite $L$ (different quantities will give different $T_c$)

$\gamma, \nu$ can be extracted by studying peaks in $\xi(T)$

Similarly for specific heat;

$$C_{\text{max}} \sim L^{\alpha/\nu}$$
Susceptibility: \[ \chi = \frac{1}{N} \frac{1}{T} (\langle M^2 \rangle - \langle |M| \rangle^2) \]

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)
General finite-size scaling hypothesis

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

Test this finite-size scaling form

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

What is the exponent $\sigma$?

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

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

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

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

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 $t L^{1/\nu}$
2D Ising model; \( \gamma = 7/4, \quad \nu = 1 \)

\[ T_c = \frac{2}{\ln(1 + \sqrt{2})} \approx 2.2692 \]

In general; find \( T_c \) and exponents so that large-\( L \) curves scale
Binder ratio \[ Q = \frac{\langle m^2 \rangle}{\langle |m| \rangle^2} \]

Useful dimensionless quantity for accurately locating Tc

Infinite-size behavior:
\[ \langle m^2 \rangle \sim t^{-\gamma} \]
\[ \langle |m| \rangle \sim t^{-\gamma/2} \]

Implies finite-size scalings
\[ \langle m^2 \rangle \sim L^{\gamma/\nu} \]
\[ \langle |m| \rangle \sim L^{\gamma/2\nu} \]

Hence Q should be size-independent at the critical point
\[ Q \rightarrow 1 \quad \text{for} \quad T \rightarrow 0, \quad Q \rightarrow \text{constant} \quad \text{for} \quad T \rightarrow \infty \]

Q(L) curves for different L cross at Tc; often small corrections
Binder ratio: \[ Q = \frac{\langle m^2 \rangle}{\langle |m| \rangle^2} \]

Q is size independent at Tc (useful for locating Tc)
Crossing points for, e.g., sizes $L$, $2L$ can be extrapolated to infinite $L$ to give an accurate value for $T_c$ - in many cases: sufficient accuracy for two large sizes.
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

$$A_Q(\tau) = \frac{\langle Q_{i+\tau} Q_i \rangle - \langle Q_i \rangle^2}{\langle Q_i^2 \rangle - \langle Q_i \rangle^2}$$

(time averages)

Asymptotical decay

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

Integrated autocorrelation time

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

Critical slowing down

$$\Theta \to \infty \text{ as } T \to T_c$$

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

$$\Theta \sim L^z, \quad z = \text{dynamic exponent}$$
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 $tobs(K)$; first $k$ steps to fill the vector. Then, shift values after each step, add latest measurement:

\[
\begin{align*}
\text{vector contents after MC step } n & \\
Q_n & Q_{n-1} & Q_{n-2} & \ldots & \ldots & \ldots & Q_{n-K+1} \\
\text{vector contents after MC step } n+1 & \\
Q_{n+1} & Q_n & Q_{n-1} & \ldots & \ldots & \ldots & Q_{n-K+2}
\end{align*}
\]

Accumulate time-averaged correlation functions

\[
\begin{align*}
do & \ t = 2, k \\
& \quad tobs(t) = tobs(t-1) \\
enddo \\
tobs(1) &= q \\
do & \ t = 0, k - 1 \\
& \quad acorr(t) = acorr(t) + tobs(1) \times tobs(1 + t) \\
enddo
\]
2D Ising autocorrelation functions for $|M|$ 

$T/J=3.0 > T_c$

Exponentially decaying autocorrelation function
- convergent autocorrelation time
$T/J = 2.269 = T_c$

Autocorrelation time diverges with $L$
Critical slowing down

Dynamic exponent $Z$: $\Theta, \Theta_{\text{int}} \sim L^Z$

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