Statistical errors ("error bars")

Calculation based on M "bins". What is the statistical error? Consider M independent calculations (each based on n configs)

Statistically independent averages $\bar{A}_i, \ i = 1, \ldots, M$

Full average

$$\bar{A} = \frac{1}{M} \sum_{i=1}^{M} A_i$$

Standard deviation

$$\sigma' = \sqrt{\frac{1}{M} \sum_{i=1}^{M} (\bar{A}_i^2 - \bar{A}^2)}$$

But, we want the standard deviation of the average

$$\sigma = \sqrt{\frac{1}{M(M-1)} \sum_{i=1}^{M} (\bar{A}_i^2 - \bar{A}^2)}$$

The bins have to be long enough (\# of MC steps, n, large enough) to be essentially statistically independent (can be quantified by "autocorrelations" - later)
Squared magnetization for different system sizes (no external field): development of phase transition
Finite-size scaling

\[ T > T_c : \langle M^2 \rangle \to 0 \text{ (as } 1/L^2, \text{ trivial from short-range correlations)} \]
\[ T = T_c : \langle M^2 \rangle \to 0 \text{ (non-trivial power law)} \]
\[ T < T_c : \langle M^2 \rangle \to \text{ constant }> 0 \]

Extracting an exponent: \[ A = aL^\alpha \to \ln(A) = \ln(a) + \alpha \ln(L) \]
- Power-law: straight line when plotted on log-log scale
- The \( 1/L^2 \) form for \( T/J=2.5 \) not yet seen because of cross-over behavior; close to the critical point, larger \( L \) required
Critical behavior and scaling

Correlation length $\xi$ 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

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

$\nu$ 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 $T < T_c$ (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

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

Singular at $T_c$

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

The exponent $\alpha$ can be positive or negative (no divergence
If negative; 0 can correspond to log divergence)
Magnetization of 2D Ising ferromagnet

\[ \langle |m| \rangle \sim (T_c - T)^\beta, \quad (T < T_c) \text{ for infinite system} \]
Magnetization squared $\langle m^2 \rangle \sim (T_c - T)^{2\beta}$, \quad ($T < T_c$)

The exponent $\beta$ can be extracted for large $L$. 
Comparison with known 2D Ising model exponent

\[ \beta = \frac{1}{8} \]

If \( T_c \) 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 $\xi \to L$

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

At what $T$ does the maximum occur?

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

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)