The Monte Carlo trick

\[ I = \int_D g(x) \, dx \]

iid random samples uniformly drawn from \( D \)

\[ \hat{I}_m = \frac{1}{m} \left( g(x^{(1)}) + \cdots + g(x^{(m)}) \right) \]

law of the large numbers

\[ P \left[ \lim_{m \to \infty} |\hat{I}_m - I| = 0 \right] = 1 \]
The Monte Carlo trick

central limit theorem

\[ \lim_{m \to \infty} \text{Cdf} \sqrt{m} \left( \hat{I}_m - I \right) = \text{Cdf} \mathcal{N}(0, \sigma^2) \]

convergence is

\[ \mathcal{O}(m^{-1/2}) \]

regardless of the dimensionality of \( D \)
Importance sampling

\[ I = \int_{0}^{\infty} g(x) e^{-x} \, dx \]

draw exponentially distributed random numbers, then

\[ \hat{I}_m = \frac{1}{m} \left( g(x^{(1)}) + \cdots + g(x^{(m)}) \right) \]

how?

\[ u \in [0, 1] \]

standard random number generator

\[ p = -\ln u \quad \rightarrow \quad p \in [0, \infty] \]

inverse transformation is needed
Importance sampling

Statistical mechanics:

\[ \langle Q \rangle = \frac{1}{Z} \text{Tr} \left[ Q e^{-\beta H} \right] = \frac{\text{Tr}[Q e^{-\beta H}]}{\text{Tr}[e^{-\beta H}]} \]

unnormalized weights

\[ W(x) = e^{-\beta E(x)} \]

how do we get random variables that are distributed according to \( W(x) \) ?
Independent sampling

Known geometry converges to $\pi/4$
Markov chains and rejections

Small steps random walk through configuration space at each time: measure

Rejection: stay at same configuration, update clock and measure
A Markov chain is a sequence of random variables $X_1, X_2, X_3, \ldots$ with the property that the future state depends only on the past via the present state.

$$P[X_{n+1} = x | X_n = x_n, \ldots, X_1 = x_1, X_0 = x_0] = P[X_{n+1} = x | X_n = x_n]$$

**transition function**

$$T(x, y)$$

$$\sum_{y} T(x, y) = 1$$

**conservation of probability**
Markov chains

- irreducible
- aperiodic

\[
\text{transition kernel has one eigenvalue } 1, \\
\text{while all other eigenvalues satisfy } |\lambda_j| < 1, j = 2, \ldots, N
\]

The second largest eigenvalue determines the correlations in the Markov process
Detailed balance

A transition rule $T(x,y)$ leaves the target distribution $W(x)$ invariant if

$$\sum_{x} W(x)T(x,y) \sim W(y)$$

This will certainly be the case if detailed balance is fulfilled,

$$W(x)T(x,y) = W(y)T(y,x)$$
we cannot construct a transition kernel $T$ that fulfills detailed balance.

proposal function $P(x, y)$

acceptance factor

$q = \min \left[ 1, \frac{W(y)P(y, x)}{W(x)P(x, y)} \right]$
Thermalization

energy landscape

Initial configuration

$|\lambda_2|$

$
\lambda_2
$

$\tau_{int}$

Discard the first 20% of the Markov steps!

Markov Chain should be sufficiently long
Binning analysis

- Markov chain correlates measurements
- If chain is long enough, then the configuration is independent of the initial one

\[ \tau_{\text{int}}(l) = \frac{l\sigma^2(l)}{2\sigma^2} \]

Identically and independent
Jackknife

$R^{(j)}$, $j = 1, k$

Bias = $(k-1)(R^\text{av} - R^{(0)})$

$R = R^{(0)} - \text{Bias}$

$\delta R = \sqrt{k - 1} \left( \frac{1}{k} \sum_{j} (R^{(j)})^2 - (R^\text{av})^2 \right)^{1/2}$
Ising model

\[ H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \]

Select random spin

\[ P(x, y) = P(y, x) = \frac{1}{L^2} \]

\[ \frac{W(y)}{W(x)} = \exp \left( -2\beta J \sigma_i \sum_{\langle i,j \rangle} \sigma_j \right) \]

\[ q = \min \left[ 1, \frac{W(y)P(y, x)}{W(x)P(x, y)} \right] \]

\[ q = \min \left[ 1, e^{-2\beta J \sigma_i \sum_{\langle i,j \rangle} \sigma_j} \right] \]
Critical slowing down

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

Magnetization

\[ \Delta m = \pm 2 \]

divergence of correlation length, critical fluctuations
Cluster method (Wolff)

select like spins with probability $p$

$$p = 1 - \exp[-2\beta]$$

then update always accepted
### Phase transition

#### Error on magnetization

![Error on magnetization graph](image)

#### Cluster size in Wolff

![Cluster size in Wolff graph](image)

### Functional forms and exponents

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Functional form</th>
<th>Exponent</th>
<th>Ising $d = 2$</th>
<th>Ising $d = 3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>magnetization</td>
<td>$m \propto (T_c - T)^\beta$</td>
<td>$\beta$</td>
<td>$1/8$</td>
<td>$0.3258(44)$</td>
</tr>
<tr>
<td>susceptibility</td>
<td>$\chi \propto</td>
<td>T - T_c</td>
<td>^{-\gamma}$</td>
<td>$\gamma$</td>
</tr>
<tr>
<td>correlation length</td>
<td>$\xi \propto</td>
<td>T - T_c</td>
<td>^{-\nu}$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>specific heat</td>
<td>$C(T) \propto</td>
<td>T - T_c</td>
<td>^{-\alpha}$</td>
<td>$\alpha$</td>
</tr>
<tr>
<td>inverse critical temp.</td>
<td>$1/T_c$</td>
<td></td>
<td>$\frac{1}{2} \ln(1 + \sqrt{2})$</td>
<td>$0.221657(2)$</td>
</tr>
</tbody>
</table>
Thanks!