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:

```
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
```
Cluster algorithm for the Ising model

Define bond index corresponding to pair of interacting spins

$$\text{bond } b = 1, 2, \ldots, N_b, \text{ interacting spins } \sigma_{i(b)}, \sigma_{j(b)}$$

Number of bonds $N_b = dN$ for a d-dimensional cubic lattice

Write the energy of the Ising ferromagnet as

$$E = -|J| \sum_{b=1}^{N_b} [\sigma_{i(b)} \sigma_{j(b)} + 1] = - \sum_{b=1}^{N_b} E_b$$

Write the partition function as

$$Z = \sum_{\sigma} e^{-E(\sigma)/T} = \sum_{\sigma} \prod_{b=1}^{N_b} e^{E_b/T} = \sum_{\sigma} \prod_{b=1}^{N_b} [1 + (e^{E_b/T} - 1)]$$

Define bond functions with arguments 0,1 (bond variable):

$$F_b(0) = 1$$
$$F_b(1) = e^{E_b/T} - 1$$

$$Z = \sum_{\sigma} \prod_{b=1}^{N_b} [F_b(0) + F_b(1)]$$
Introduce bond variables
\[ \tau_b = 0, 1, \quad \tau = \{\tau_1, \tau_2, \ldots, \tau_{N_b}\} \]
Partition function can be written as sum over spins and bonds
\[ Z = \sum_{\sigma} \prod_{b=1}^{N_b} [F_b(0) + F_b(1)] = \sum_{\sigma} \sum_{\tau} \prod_{b=1}^{N_b} F_b(\tau_b) \]
The functions \( F_b \) depend on the spins:
\[ \begin{align*}
F_b(0) &= 1 \\
F_b(1) &= e^{E_b/T} - 1 = \begin{cases} 
 e^{2|J|/T} - 1, & \text{if } \sigma_i(b) = \sigma_j(b) \\
 0, & \text{if } \sigma_i(b) \neq \sigma_j(b)
\end{cases}
\]
\( \tau_b = 1 \) allowed only between parallel spins
Probabilities: For everything else fixed, probability for a given \( b \)
\[ P(\tau_b) = \frac{F(\tau_b)}{F(0) + F(1)} = \frac{F(\tau_b)}{e^{2|J|/T}} \]
If parallel spins on bond \( b \), probabilities for the bond variable
\[ P(\tau_b = 0) = e^{-2|J|/T}, \quad P(\tau_b = 1) = 1 - e^{-2|J|/T} \]
If anti-parallel spins on bond \( b \)
\[ P(\tau_b = 0) = 1, \quad P(\tau_b = 1) = 0 \]
For a fixed bond configuration, spins forming clusters (spins connected by “filled” bonds) can be flipped and then give a configuration (term) with the same weight in Z ($F_b=1$ for all bonds between clusters, $F_b$ unchanged inside cluster).

\[ N(\tau_b = 1) = \text{No. of filled bonds} \]
\[ W = (e^{2|J|/T} - 1)^{N(\tau_b=1)} \] (unchanged after flip)

Spins not connected to any filled bonds are single-spin clusters

**Swendsen-Wang algorithm**
- Start from spin configuration
- Generate bond configuration
- Identify clusters of spins connected by bonds
- Flip each cluster with probability 1/2
- Generate new bonds with the current spins, etc
$T = 3.00$
$T = 2.00$
Integrated autocorrelation times
- $z=0$ for Swendsen-Wang in two dimensions?
- log-divergence of autocorrelation time?
- More likely $z \sim 0.3$ (hard to distinguish $L^z$ and log if $z$ small)
Cluster finding/flipping

Clusters can be constructed and flipped in the same process

1. Decide whether or not to flip (50% probability) before starting

2. Store array with flags for spins visited

   - Start with spin that has not been visited; seed of cluster
   - Add connected (by filled bonds) neighbors to cluster
   - Examine the non-visited neighbors of the new spins added
   - Add connected neighbors to cluster
   - Until no more spins in the cluster with non-visited neighbors

Use stack to store spins with neighbors to be examined