Exact computation for Ising model

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We calculate exact solution by finding the exact value of the partition function

$$Z(\beta) \quad = \sum_{\{\text{all configurations } \sigma_i\}} e^{-\beta E(\sigma_1, \sigma_2, \ldots, \sigma_n)}.$$

To do that we have to evaluate all possible configurations of spins. For given number n of spins on the lattice we have 2^n configurations. For example for two spins chain we have

$$\{\uparrow\uparrow, \downarrow\uparrow, \uparrow\downarrow, \downarrow\downarrow\} \quad .$$

Note that some of those configurations may have the same energy E, thus Z function can be written in a bit different way

$$Z(\beta) = \sum_{E_i} N(E_i) e^{-\beta E_i}, \tag{1}$$

where the sum runs over all possible energies E_i, and $N(E_i)$ is density of states: number of states with the same energy E_i.

To generate $N(E)$ we have to calculate E for all configurations of spins. In order to do that we use Gray code enumeration of spins (the description of the algorithm can be found e.g. in textbook: *Statistical Mechanics Algorithms and Computations*, Werner Krauth). The pseudo-code of the algorithm is following:

procedure `gray-flip`
input $\{\tau_0, \ldots, \tau_N\}$
$k \leftarrow \tau_0$
if $(k > N)$ **exit**
$\tau_{k-1} \leftarrow \tau_k$
$\tau_k \leftarrow k + 1$
if $(k \neq 1)$ $\tau_0 \leftarrow 1$
output $k, \{\tau_0, \ldots, \tau_N\}$
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Figure 1: Gray code for spins $\{1, ..., N\}$. The procedure returns k which is the index of next spin to flip. τ is an auxiliary vector used by the procedure. The initial value of $\tau_i = i$. Look in the code to see how to use it in practice.

Having the $N(E)$ allows us to calculate all properties of the system from (1). As an example we calculated plots of specific heat C_V in function of temperature T. The specific heat is given by expression

$$C_V = \frac{\partial \langle E \rangle}{\partial T},$$

where $\langle E \rangle = -\frac{\partial \log(Z)}{\partial \beta} = T^2 \frac{\partial \log(Z)}{\partial T}$. Thus we have

$$C_V = 2T \frac{\partial \log(Z)}{\partial T} + T^2 \frac{\partial^2 \log(Z)}{\partial T^2}.$$

For simplicity we calculate C_V using numerical differentiation using the finite difference method, which leads to following approximation

$$\begin{aligned} C_V \quad (T) \approx & \quad 2T \left(\frac{\log\left(Z(T + \Delta T)\right) - \log\left(Z(T - \Delta T)\right)}{2\Delta T} \right) \\ + & \quad T^2 \left(\frac{\log\left(Z(T + \Delta T)\right) + \log\left(Z(T - \Delta T)\right) - 2\log\left(Z(T)\right)}{\Delta T^2} \right). \end{aligned}$$

We choose small value of $\Delta T = 0.01$ which should give us accurate approximation of C_V.

Note that this approach gives us exact solution to 2D Ising model, but it is limited to very small lattice sizes. The bottleneck of the algorithm is the part where we calculate $N(E)$ using Gray code. This is because we have to run over 2^n states which for lattice of size 6×6 gives $2^{36} = 68719476736$ number of possible configurations.