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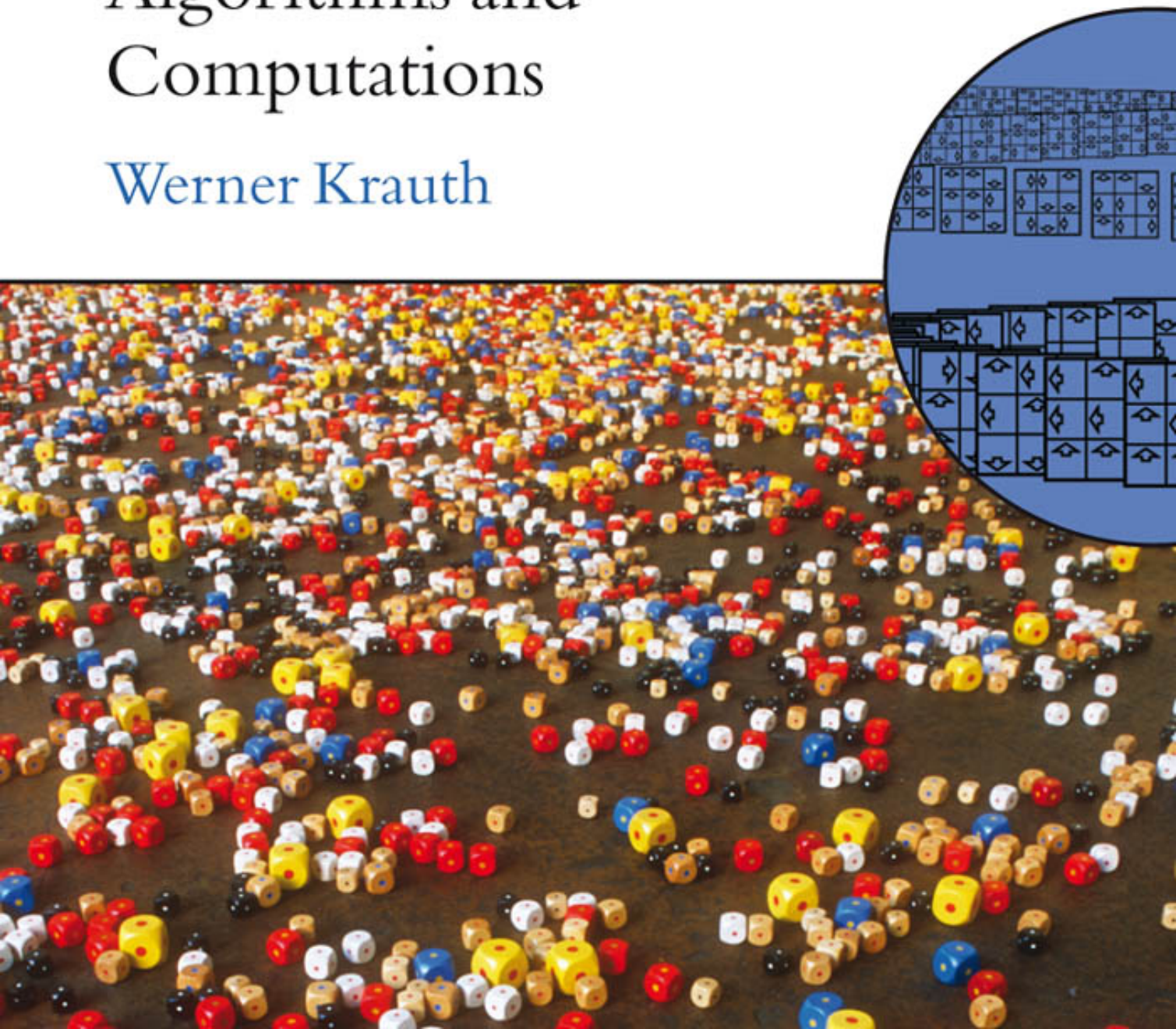
Statistical Mechanics:

Algorithms and Computations

Werner Krauth



Statistical Mechanics

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5.1 The Ising model—exact computations

The Ising model describes spins $\sigma_k \pm 1$, $k = 1, \ldots, N$, on a lattice, for example the two-dimensional square lattice shown in Fig. 5.1. In the simplest case, the ferromagnetic Ising model, neighboring spins prefer to align. This means that pairs $\{+,+\}$ and $\{-,-\}$ of neighboring spins direction have a lower energy than antiparallel spins (pairs $\{+,-\}$ and $\{-,+\}$), as expressed by the energy

$$E = -J \sum_{\langle k,l \rangle} \sigma_k \sigma_l. \tag{5.1}$$

The sum is over all pairs of neighbors. The parameter J is positive, and we shall take it equal to one. In a two-dimensional square lattice, the sites k and l then differ by either a lattice spacing in x or a lattice spacing in y. In a sum over pairs of neighbors, as in eqn (5.1), we consider each pair only once, that is, we pick either $\langle k,l \rangle$ or $\langle l,k \rangle$. Algorithm 5.1 (`energy-ising`) implements eqn (5.1) with the help of a neighbor scheme that we have encountered already in Chapter 1. The sum n runs over half the neighbors, so that each pair $\langle l,k \rangle$ is indeed counted only once. We shall soon adopt better approaches for calculating the energy, but shall always keep Alg. 5.1 (`energy-ising`) for checking purposes. We also note that the lattice may either have periodic boundary conditions or be planar.

procedure `energy-ising`
input $\{\sigma_1, \ldots, \sigma_N\}$
$E \leftarrow 0$
for $k = 1, \ldots, N$ **do**
  for $n = 1, \ldots, d$ **do** (d: space dimension)
    $j \leftarrow \mathrm{Nbr}(n,k)$
    if $(j \neq 0)$ **then**
      $E \leftarrow E - \sigma_k \sigma_j$
output E

Algorithm 5.1 `energy-ising`. Computing the energy of an Ising-model configuration. Nbr(.,.) encodes the neighbor scheme of Fig. 5.2.

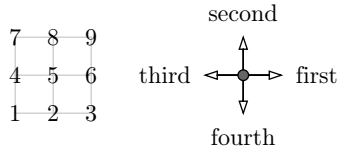


Fig. 5.2 Neighbor scheme in the two-dimensional Ising model. The first neighbor of 2 is $\mathrm{Nbr}(1,2) = 3$, $\mathrm{Nbr}(4,2) = 0$, etc.

The Ising model's prime use is for magnets. Figure 5.1, however, illustrates that it can also serve to describe particles on a lattice. Now, a variable $\tilde{\sigma}_k = 1, 0$ signals the presence or absence of a particle on site k. Let us suppose that particles prefer to aggregate: two particles next to each other have a lower energy than two isolated particles. The simplest configurational energy is

$$E = -4\tilde{J} \sum_{\langle k,l \rangle} \tilde{\sigma}_k \tilde{\sigma}_l.$$

However, the transformation $\tilde{\sigma}_k = \frac{1}{2}(\sigma_k + 1)$ brings us back to the original Ising model.

The main difference between the Ising model considered as a magnet and as a lattice gas is in the space of configurations: for a magnet, the spins can be up or down, more or less independently of the others, so that all of the 2^N configurations $\{\sigma_1, \ldots, \sigma_N\} = \{\pm 1, \ldots, \pm 1\}$ contribute to the partition function. For the lattice gas, the number of particles, equivalent to the proportions of up and down spins, must be kept constant, and the partition function is made up of all configurations with a fixed $M = \sum_k \sigma_k$. For large N, the two versions of the Ising model become more or less equivalent: it is sufficient to include a constant external magnetic field, which plays the same role here as the chemical potential in Section 4.1.3.

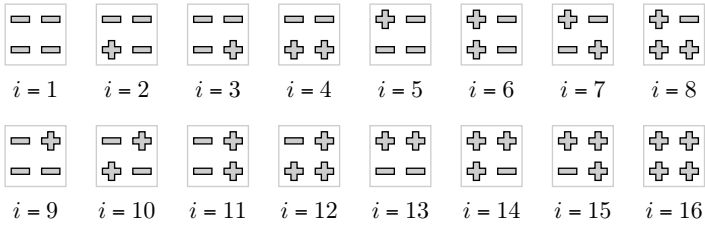


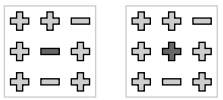
Fig. 5.3 List of configurations of the Ising model on a 2×2 square lattice.

In Fig. 5.3, we list all configurations for a (magnetic) Ising model on a 2×2 lattice. Without periodic boundary conditions, configurations $i = 1$ and $i = 16$ have an energy $E = -4$, and configurations $i = 7$ and $i = 10$ have an energy $E = +4$. All others are zero-energy configurations.

5.1.1 Listing spin configurations

In the present subsection, we enumerate all the spin configurations of the Ising model; in fact, we list them one after another. Most simply, each configuration $i = 1, \ldots, 2^N$ of N Ising spins is related to the binary representation of the number $i - 1$: in Fig. 5.3, zeros in the binary representation of $i - 1$ correspond to down spins, and ones to up spins. As an example, the binary representation of the decimal number 10 (configuration $i = 11$ in Fig. 5.3) is 1010, which yields a spin configuration $\{+, -, +, -\}$ to be translated to the lattice with our standard numbering scheme. It is a simple matter to count numbers from 0 to $2^N - 1$ if N is not too large, to represent each number in binary form, and to compute the energy and statistical weight $\mathrm{e}^{-\beta E}$ of each configuration with Alg. 5.1 (`energy-ising`).

It is often faster to compute the change of energy resulting from a spin-flip rather than the energy itself. In Fig. 5.4, for example, we can find out that $E_b = E_a - 4$, simply because the "molecular field" acting on the central site is equal to 2 (it is generated by three up spins and one down spin). The change in energy is equal to twice the value of the spin at the site times the molecular field.



a *b*

Fig. 5.4 Two configurations of the Ising model connected by the flip of a single spin.

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 $k, \{\tau_0, \ldots, \tau_N\}$

Algorithm 5.2 `gray-flip`. Gray code for spins $\{1, \ldots, N\}$. k is the next spin to flip. Initially, $\{\tau_0, \ldots, \tau_N\} = \{1, \ldots, N + 1\}$.

On lattices of any size, the change in energy can be computed in a constant number of operations, whereas the effort for calculating the energy grows with the number of edges. Therefore it is interesting that all 2^N spin configurations can be enumerated through a sequence of 2^N spin-flips, one at a time. (Equivalently, one may enumerate all numbers $\{0, \ldots, 2^N - 1\}$ by changing a single digit at a time during the enumeration.) Algorithms that perform such enumerations are called Gray codes, and an application of a Gray code for four spins is shown in Table 5.1. How it works can be understood by (mentally) folding Table 5.1 along the horizontal line between configurations $i = 8$ and $i = 9$: the configurations of the first three spins $\{\sigma_1, \sigma_2, \sigma_3\}$ are folded onto each other (the first three spins are the same for $i = 8$ and $i = 9$, and also for $i = 7$ and $i = 10$, etc.). The spins $\{\sigma_1, \sigma_2, \sigma_3\}$ remain unchanged between $i = 8$ and $i = 9$, and this is the only moment at which σ_4 flips, namely from $-$ to $+$. To write down the Gray code for $N = 5$, we would fold Table 5.1 along the line following configuration $i = 16$, and insert $\{\sigma_5(i = 1), \ldots, \sigma_5(i = 16)\} = \{-, \ldots, -\}$, and $\{\sigma_5(i = 17), \ldots, \sigma_5(i = 32)\} = \{+, \ldots, +\}$. Algorithm 5.2 (`gray-flip`) provides a practical implementation. We may couple the Gray code enumeration to an update of the energy (see Alg. 5.3 (`enumerate-ising`)). Of course, the Gray code still has exponential running time, but the enumeration as in Fig. 5.5 gains a factor $\propto N$ with respect to naive binary enumeration.

Algorithm 5.3 (`enumerate-ising`) does not directly compute the partition function at inverse temperature β, but rather the number of configurations with energy E, in other words, the density of states $\mathcal{N}(E)$

Table 5.1 Gray-code enumeration of spins $\{\sigma_1, \ldots, \sigma_4\}$. Each configuration differs from its predecessor by one spin only.

i	$\{\sigma_1, \ldots, \sigma_4\}$			
1	$-$	$-$	$-$	$-$
2	$+$	$-$	$-$	$-$
3	$+$	$+$	$-$	$-$
4	$-$	$+$	$-$	$-$
5	$-$	$+$	$+$	$-$
6	$+$	$+$	$+$	$-$
7	$+$	$-$	$+$	$-$
8	$-$	$-$	$+$	$-$
9	$-$	$-$	$+$	$+$
10	$+$	$-$	$+$	$+$
11	$+$	$+$	$+$	$+$
12	$-$	$+$	$+$	$+$
13	$-$	$+$	$-$	$+$
14	$+$	$+$	$-$	$+$
15	$+$	$-$	$-$	$+$
16	$-$	$-$	$-$	$+$

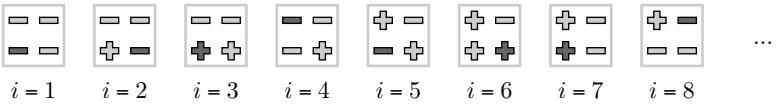


Fig. 5.5 List of Ising-model configurations on a 2×2 square lattice, generated by the Gray code (only the dark spins flip, see Table 5.1).

procedure `enumerate-ising`
$\{\mathcal{N}(-2N), \ldots, \mathcal{N}(2N)\} \leftarrow \{0, \ldots, 0\}$
$\{\sigma_1, \ldots, \sigma_N\} \leftarrow \{-1, \ldots, -1\}$
$\{\tau_0, \ldots, \tau_N\} \leftarrow \{1, \ldots, N+1\}$
$E \leftarrow -2N$
$\mathcal{N}(E) \leftarrow 2$
for $i = 1, \ldots, 2^{N-1} - 1$ **do**
$k \leftarrow$ `gray-flip` $(\{\tau_0, \ldots, \tau_N\})$
$h \leftarrow \sum_{\langle j,k \rangle} \sigma_j$ (field on site k)
$E \leftarrow E + 2 \cdot \sigma_k h$
$\mathcal{N}(E) \leftarrow \mathcal{N}(E) + 2$
$\sigma_k \leftarrow -\sigma_k$
output $\{\mathcal{N}(E) > 0\}$

Algorithm 5.3 `enumerate-ising`. Single spin-flip (Gray code) enumeration for the Ising model, using Alg. 5.2 (`gray-flip`).

Table 5.2 Density of states $\mathcal{N}(E)$ for small square lattices with periodic boundary conditions (from Alg. 5.3 (`enumerate-ising`))

	$\mathcal{N}(E) = \mathcal{N}(-E)$		
E	2×2	4×4	6×6
0	12	20 524	13 172 279 424
4	0	13 568	11 674 988 208
8	2	6 688	8 196 905 106
12	.	1 728	4 616 013 408
16	.	424	2 122 173 684
20	.	64	808 871 328
24	.	32	260 434 986
28	.	0	71 789 328
32	.	2	17 569 080
36	.	.	3 846 576
40	.	.	804 078
44	.	.	159 840
48	.	.	35 148
52	.	.	6 048
56	.	.	1 620
60	.	.	144
64	.	.	72
68	.	.	0
72	.	.	2

(see Table 5.2). We must take care in implementing this program because $\mathcal{N}(E)$ can easily exceed 2^{31}, the largest integer that fits into a standard four-byte computer word. We note, in our case, that it suffices to generate only half of the configurations, because $E(\sigma_1, \ldots, \sigma_N) = E(-\sigma_1, \ldots, -\sigma_N)$.

5.1.2 Thermodynamics, specific heat capacity, and magnetization

The Ising-model partition function $Z(\beta)$ can be obtained by summing appropriate Boltzmann factors for all configurations, but it is better to start from the density of states, the number of configurations with energy E, as just calculated:

$$Z(\beta) = \overbrace{\sum_{\sigma_1 = \pm 1, \ldots, \sigma_N = \pm 1} \mathrm{e}^{-\beta E(\sigma_1, \ldots, \sigma_N)}}^{\propto 2^N \text{ terms}} = \overbrace{\sum_E \mathcal{N}(E)\, \mathrm{e}^{-\beta E}}^{\propto N \text{ terms}} .$$

Similarly, the mean energy $\langle E \rangle$ can be computed from $Z(\beta)$ by numerical differentiation, that is,

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log Z, \tag{5.2}$$

but we are again better off using an average over the density of states:

$$\langle E\rangle = \frac{\sum_{\boldsymbol{\sigma}} E_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}} = \frac{1}{Z}\sum_{E} E\mathcal{N}(E)\,\mathrm{e}^{-\beta E}, \tag{5.3}$$

where we have used $\boldsymbol{\sigma}$ as a shorthand for $\{\sigma_1, \ldots, \sigma_N\}$. Higher moments of the energy can also be expressed via $\mathcal{N}(E)$:

$$\left\langle E^2\right\rangle = \frac{\sum_{\boldsymbol{\sigma}} E_{\boldsymbol{\sigma}}^2 \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}} = \frac{1}{Z}\sum_{E} E^2\mathcal{N}(E)\,\mathrm{e}^{-\beta E}. \tag{5.4}$$

The specific heat capacity C_V, the increase in internal energy caused by an infinitesimal increase in temperature,

$$C_V = \frac{\partial\langle E\rangle}{\partial T} = \frac{\partial\beta}{\partial T}\frac{\partial\langle E\rangle}{\partial\beta} = -\beta^2\frac{\partial\langle E\rangle}{\partial\beta}, \tag{5.5}$$

can be expressed via eqn (5.2) as a second-order derivative of the partition function:

$$C_V = \beta^2\frac{\partial^2}{\partial\beta^2}\log Z.$$

Again, there is a more convenient expression, which we write for the specific heat capacity per particle c_V,

$$\underline{c_V} = -\frac{\beta^2}{N}\frac{\partial\langle E\rangle}{\partial\beta} = -\frac{\beta^2}{N}\frac{\partial}{\partial\beta}\left(\frac{\sum_{\boldsymbol{\sigma}} E_{\boldsymbol{\sigma}}\mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}}{\sum_{\boldsymbol{\sigma}}\mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}}\right)$$
$$= \frac{\beta^2}{N}\frac{\sum_{\boldsymbol{\sigma}} E^2\mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}\sum_{\boldsymbol{\sigma}}\mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}} - \left(\sum_{\boldsymbol{\sigma}} E_{\boldsymbol{\sigma}}\mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}\right)^2}{\left(\sum_{\boldsymbol{\sigma}}\mathrm{e}^{-\beta E_{\boldsymbol{\sigma}}}\right)^2} = \underline{\frac{\beta^2}{N}\left(\left\langle E^2\right\rangle - \langle E\rangle^2\right)},$$

which can be evaluated with the second formulas in eqns (5.3) and (5.4) and is implemented in Alg. 5.4 (`thermo-ising`). We can recognize that the specific heat capacity, an experimentally measurable quantity, is proportional to the variance of the energy, a statistical measure of the distribution of energies. Specific-heat-capacity data for small two-dimensional lattices with periodic boundary conditions are shown in Fig. 5.6.

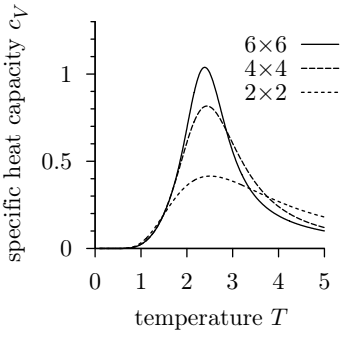


Fig. 5.6 Specific heat capacity of the Ising model on small square lattices with periodic boundary conditions (from Alg. 5.4 (`thermo-ising`)).

The density of states $\mathcal{N}(E)$ does not carry complete information about the Ising model. We must modify Alg. 5.3 (`enumerate-ising`) in a straightforward way to track the magnetization $M = \left\langle\sum_{k=1}^{N}\sigma_k\right\rangle$ of the system and to find the probability π_M. This probability is obtained, at any temperature, from the density of states as a function of energy and magnetization, $\mathcal{N}(E, M)$ (see Fig. 5.7). The probability distribution of the magnetization per spin is always symmetric around $M/N = 0$, featuring a single peak at $M = 0$ at high temperature, where the system is paramagnetic, and two peaks at magnetizations $\pm\tilde{M}/N$ at low temperature, where the system is in the ferromagnetic state. The critical temperature,

$$T_\mathrm{c} = \frac{2}{\log\left(1+\sqrt{2}\right)} = 2.269 \quad (\beta_\mathrm{c} = 0.4407), \tag{5.6}$$