Homework No.9

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1 Higher Dimensional Sphere

1.1 Problem Description

The interior of a d-dimensional hypersphere of unit radius is defined by the condition $x_1^2 + x_2^2 + ... + x_d^2 \leq 1$. Write a program that finds the volume of a hypersphere using a Monte Carlo method. Test your program for $d = 2$ and $d = 3$ and then calculate the volume for $d = 4$ and $d = 5$, and compare your results with the exact results.

1.2 Solution

In fact, we adopted the Hit-and-Miss method under the spirit of the Monte-Carlo approach, The integration is straightforward because the volume of a d-dimensional "hypercubic" can be calculated easily with

$$\int_{x_i \in [-\frac{a}{2}, \frac{a}{2})} d^d x_i = a^d \tag{1}$$

where $i \in 1, 2, ..., d$ and d is the number of dimension.

The volume of a hypersphere is therefore

$$\frac{n}{N} a^d \tag{2}$$

assuming there are N random number generated and n of them has a norm less than a

1.3 Output and Analysis

We first use the 3D and 2D cases to check the validity of our MC method. Sampling at 10^4 points, the volume is evaluated according to 2. We can get a theoretical result for spheres in dimensions. Just integrate in the domain where $\|x\| < a$ and the integral is

$$V_n = \frac{\pi^{n/2} R^n}{\Gamma(1 + \frac{n}{2})} \tag{3}$$

where half factorial is defined as $(\frac{n}{2})! = \frac{n}{2} \cdot (\frac{n}{2} - 1)...\frac{1}{2}\sqrt{\pi}$ Our M-C results and the theoretical results are compared in the table below:

d	V: MC	V: theory	relative error
2	3.1416	3.1416	2.5×10^{-6}
3	4.1752	4.1888	3.2×10^{-3}
4	4.8496	4.9348	1.7×10^{-2}
5	5.1200	5.2638	2.6×10^{-2}

It can be seen that the error increases as the dimension increases. I further calculate more volumes and there is a maximum in the sphere volume at $d = 5$, as is shown in 1. When the dimension is rather high, our method produces noticeable errors and I believe this can be relieved by using the sample mean method.

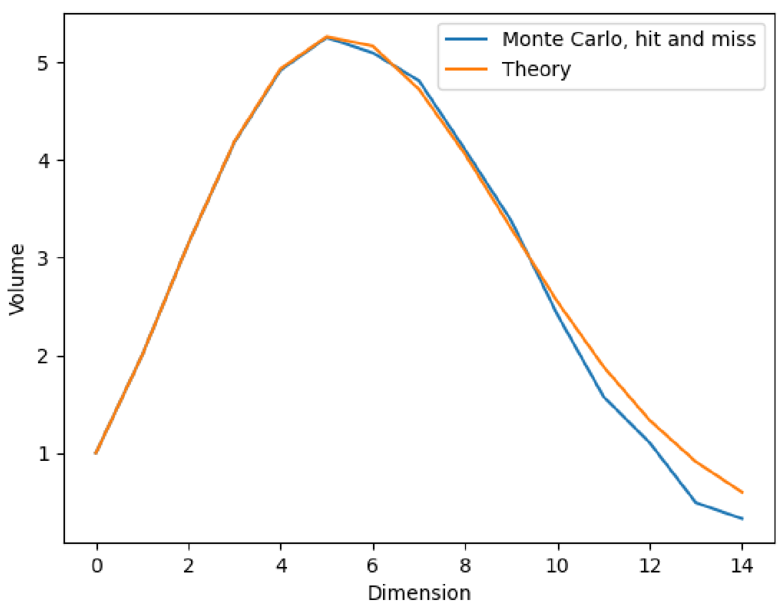

Figure 1: More hyperspheres, volume to dimension. When d larger than 10, the error is noticeable.

1.4 Pseudocode

Algorithm 1 Volume of hypersphere

Input: dimension d

Output: volume of the hypersphere calculated by the Monte-Carlo method.

```
N ← 1 × 10^4
n ← 0
for i in range(N) do
    generate a random d-dimensional vector x⃗, each component distributed linearly in [−1/2, 1/2)
    if ‖x⃗‖ < 1 then
        n ← n + 1
    end if
end for
```

Return: n/N

2 3D Classical Heisenburg Model

2.1 Problem Description

Write an MC code for a 3D Face-Centered Cubic lattice using the Heisenberg spin model (adopt periodic boundary condition). Estimate the ferromagnetic Curie temperature. The Hamiltonian is

$$H = -J \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j \tag{4}$$

where $J = 1$.

2.2 Solution

Invoking the detailed balance in statistical physics, every two states R and R' of an equilibrium system must satisfy the following criteria

$$W(R)T(R \to R') = W(R')T(R' \to R) \tag{5}$$

If we iteratively impose a random displacement to a state R and denote the changed state R', the transition probability from R to R' then becomes

$$\begin{aligned} T(R \to R') =& \frac{1}{N} \frac{W(R')}{W(R)}, \text{ if } W(R') < W(R) && (6) \\ & \frac{1}{N}, \text{ otherwise} && (7) \end{aligned}$$

The detailed balance above can actually be expressed with the canonical ensemble

$$W_R = \frac{e^{\frac{-U(R)}{k_B T}}}{\int e^{\frac{-U(r)}{k_B T}} dr} \tag{8}$$

One of the greatest benefits the Metropolis method offers is that we are freed from evaluating the partition integral in the denominator in Eq.8, for it is eliminated out in the fraction in Eq.6.

The scheme of how we adopted the Metropolis of MC is shown below:

- Choose a spin at random
- Change the selected spin at random
- Calculate the energy change introduced by the above change
- Accept the change at a probability of $e^{-\frac{\Delta E}{k_B T}}$
- loop the above steps until equilibrium is reached.

2.3 Output and Analysis

After some trials, we found that if the period is too small, or the number of *independednt* spins is small, the phase transition is hardly observable in the $\|s\| - T$ graph.

By simulating $5 \times 5 \times 5 = 125$ cells and averaging over 3 runs, our result is produced and shown in Fig.2 The Curie temperature is estimated as 3.4K.

2.4 Pseudocode

Algorithm 2 Volume of hypersphere

Output: averaged norm of spin $\|s\|$
$N_{tot} \leftarrow 1 \times 8 \times 10^4$
$N_{avg} \leftarrow 1 \times 10^2$
$S \leftarrow 0$
for i in range(N_{tot}) **do**
    randomly selects one spin $\vec{s}$
    $\vec{s_{new}} \leftarrow$ a random vector
    if $H(s_{new}) < H(s)$ **then** ▷ In fact only 12 spins coupled with the changed one are to be evaluated, using Eq4
        $s \leftarrow s_{new}$
    end if
    if $i > N_{tot} - N_{avg}$ **then**
        $S \leftarrow S+$ current averaged spin norm
    end if
end for
Return: S/N_{avg}

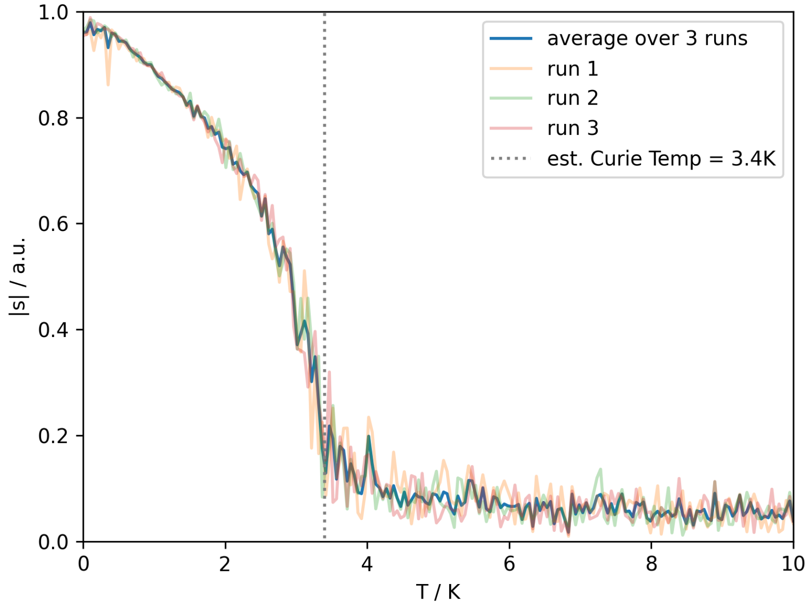

Figure 2: $\|s\|$ to T phase graph. An abrupt change in the first derivative can be seen, that is, phase transition.