Monte Carlo method and Markov chains

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TÝDEN VĚDY NA JADERCE

Abstract

This paper deals with the problem of sampling from a predetermined Boltzmann distribution (Ising model) and analyzing it to answer the given questions using Monte Carlo and Markov chains (MCMC for short). We will look at the tools we used, the way we approached the problem and the manner in which we utilized the MCMC method in our problem. Lastly, we will look at the interpretation and explanation of our results

Theoretical introduction

The Markov chain:

A Markov chain is a set of states S describing a random discrete process where the probability of a transition to the next state depends only on the current state and not on any of the previous states, (a function dependent only on x, y):

$$\mathbb{P}[X_{k+1} = y \mid X_k = x] = p(y|x)$$

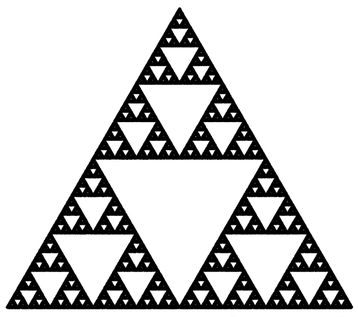

Figure 1: Sierpensky triangle generated by Markov chain

An unexpected appearance of a Sierpensky triangle

This problem is constructed by choosing a random point X_1 in a equilateral triangle ABC, and then drawing a line through this point to a random vertex A, B, C. At the centre of the newly formed line segment X_1A, X_1B, X_1C will lie a new point X_2. After a large number of repetitions of this process we get a pattern identical to the Sierpensky triangle. Note, that this is a continuous Markov chain.

Roll the dice

How many times must a person roll a die to meet all the numbers from 1-6?

The individual points on the diagram represent the number of numbers we have already rolled. The arrows show us the probability of moving to the next state. From this diagram we can already calculate the average number of throws needed to meet all numbers 1-6.

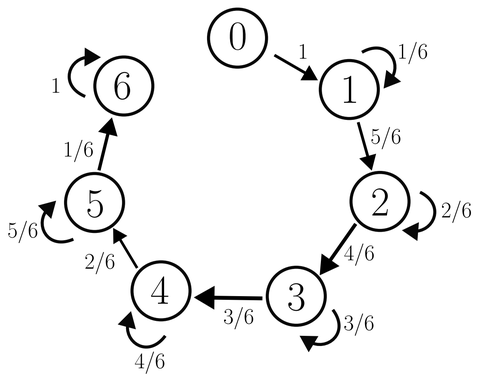

Figure 2: Markov chain of dice roll

The Monte Carlo method

Monte Carlo is a numerical method that uses data sampling and data extraction from a given distribution to determine the characteristics of the data.

$$P_X(x) \overset{\text{def}}{=} \mathbb{P}[X \leq x]$$

This is used for example in the calculation of cumulative distribution functions (CDF)

$$p_X(x) \overset{\text{def}}{=} \frac{d}{dx}(P_X(x))$$

using many unknown probability density function (PDF) values.

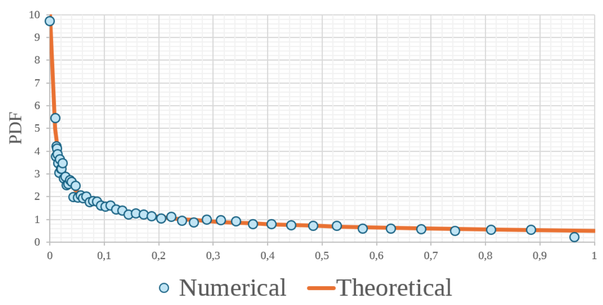

Figure 3: Distribution function

MCMC

The combination of these two methods is the MCMC (Monte Carlo Markov chain) method. To utilize this method we have to know the target $f(x)$ distribution $f(x) \propto p(x)$, up to a constant of proportionality.

Then we define an arbitrary PDF $q(x)$, and then we randomly pick a value x which will be the start of our Markov chain and subsequently we pick another value y and we calculate the transition probability using the $f(x)$ and $q(x)$ PDFs.

We define the so-called acceptance ratio, which is defined as $\min(1, \frac{f(y)q(x|y)}{f(x)q(y|x)})$

If we have calculated the acceptance ratio, we just need to generate a random number on the interval (0,1) and if the acceptance ratio is smaller, we accept y and if not, we reject.

The Simplified Ising model

Assignment

Using MCMC, we addressed our given problems in the following model: Given a space of points $\Lambda = \{0, 1, 2, \ldots, 255\}^2$

λ = a point in the grind

Can be in two states: $x(\lambda) \in \{0, 1\}$ (white or black)

Energy of a given distribution of states x: $E(x) = \sum_{\{\lambda,\lambda'\}:\|\lambda-\lambda'\|=1} |x(\lambda) - x(\lambda')|$

Relaxation distribution: $\pi(x) = \frac{1}{Z} \exp\left(-\frac{E(x)}{k_B T}\right)$

In our model we choose $k_B = 1$ and we don't need to choose Z, because the proportionality to the distribution is sufficient.

Problems to solve

1) Plot the dependence of the average energy $\bar{E}$ on temperature.
2) Let C be the number of connected black regions. Plot the dependence of the expected value of C and the temperature.
3) Let L be the probability of percolations (forming of clusters and their subsequent possibility of forming a chain connecting the top and bottom see Figure 4). We plot this value with respect to temperature.

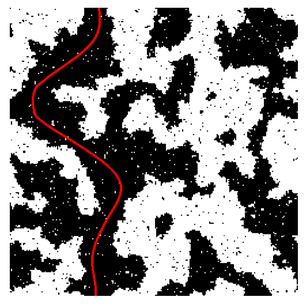

Figure 4: Percolation

Solution

We randomly generate the initial state x_0 (fifty percent chance that the box is black) and calculate its total energy. We propose the new state as follows:

Randomly select the field $\lambda_0 \in \Lambda$ and change its color, the other fields remain unchanged.

For the energy difference: $\triangle(x'|x) = E(x') - E(x) = \sum_{\lambda:\|\lambda-\lambda_0\|=1}(|x'(\lambda) - x'(\lambda_0)| - |x(\lambda) - x(\lambda_0)|)$

Acceptance ratio: $\alpha(x'|x) = \exp\left(\min\left\{0, -\frac{\triangle(x'|x)}{k_B T}\right\}\right)$

Using the process described above, it is always sufficient to accept or reject and this distribution will relax into the distribution described above.

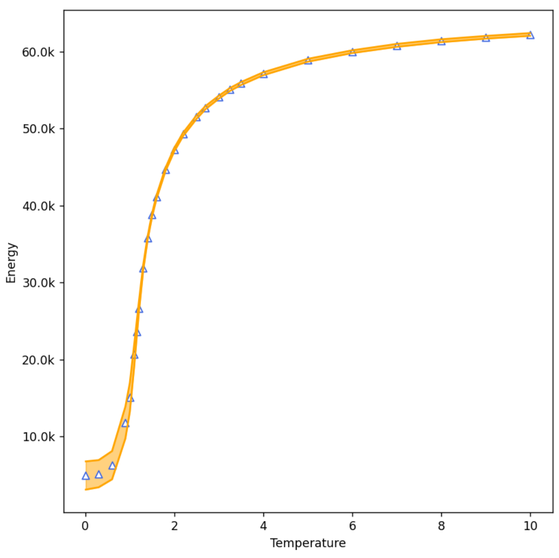

Figure 5: Steady state distributions and mean energy with temperature

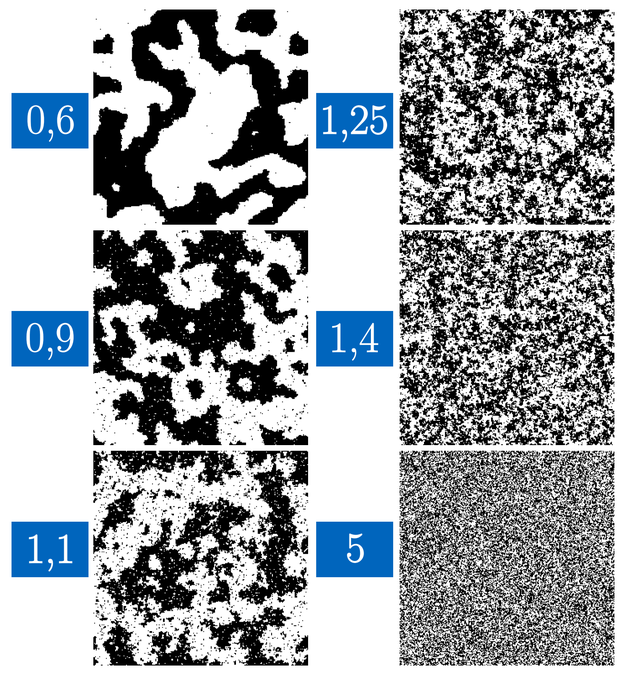

Figure 6: Development of blobs with growing temperature

Results

We processed the results by forgetting the first 10% of 10 million iterations. Individual averages are indicated by points in the graphs, the shaded areas indicate the standard deviation at each point.

In solving the first problem we obtained, using a special code, the relation in Figure 6 which shows a rapid increase in energy at the boundary of low and higher temperatures and then a much slower growth in the high and low temperatures respectively. In the second problem we attained the graph in Figure 7. We can see that the growth is very similar to the previous curve so they must be related. Lastly, in the third problem we got a much less clear result. However, we can still make out a apparent decrease in percolation probability with temperature.

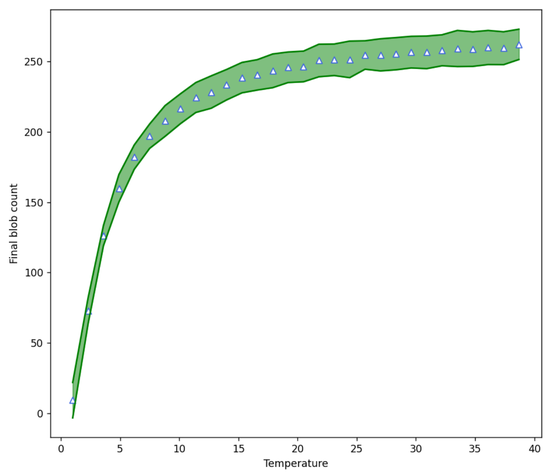

Figure 7: Number of blobs with temperature

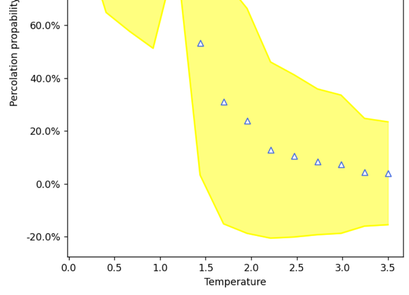

Figure 8: Percolation with temperature

Conclusion

In the first problem we saw a sudden increase in average energy and then a slowing down growth which is similar to a graph of a logarithm. The explanation is that energy in the Ising model is analagous to entropy because it is related to how the neighbours are situated around a given point and because the Boltzmann distribution will always relax to a distribution with the largest entropy (the most microstates) the energy will evolve analogously. Due to this, the number of blobs will increase in the same manner because the state with the most entropy is the one where energy between states is averagised so for small temperatures the state will be more lumpy than for bigger ones. The third one is based on the same principle with probability being the highest at the lumpy (lower) temperatures.

References

1) **Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E.** Equation of State Calculations by Fast Computing Machines. Journal of Chemical Physics, 21, 1087-1092. **(1953)**

2) **Ising, E.** Beitrag zur Theorie des Ferromagnetismus. Zeitschrift für Physik, 31, 253-258. **(1925)**

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