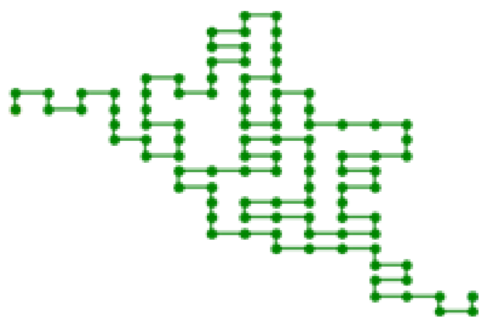
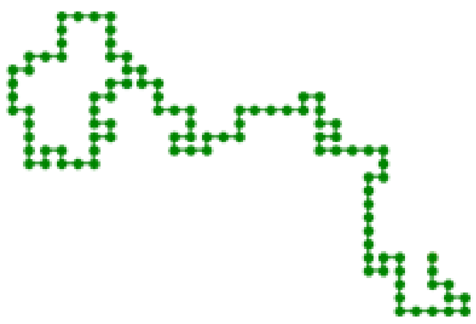
PROPERTIES OF MAGNETIC MODELS ON ENSEMBLES OF CONFORMATIONS

Introduction

Conformation is a self-avoiding random walk on a two-dimensional square grid of fixed length. Shape of the conformation depends on the temperature. There is a geometric transition between two phases: coil and globule at high and low temperatures, respectively. Looking at the examples of globule and coil conformations we can see that coils are structurally similar to one-dimensional grid and globules are similar to two-dimensional grid. From studies of the Ising model we know that magnetic phase transition appears on two-dimensional grid and does not appear on one-dimensional. So, our hypothesis is that there is a magnetic transition in globules and no transitions in coils.



globule



coil

Model

In this model, we observe sets of conformations of equal length generated at the same temperature. Each conformations generated independently as a random walk on two-dimensional grid. On each conformation we calculate Ising model, by placing a spin in each vertex of the conformation. The Hamiltonian and partiotion function is calculated by the following formula

$$H = -J \sum_{(i,j)} \sigma_i \sigma_j \qquad Z = \sum_{\{\sigma\}} e^{-H\beta}, \beta = \frac{1}{kT}$$

Where *k* is Boltzmann constant and *T* is temperature. Magnetization of a single state is a sum of spins. And magnetization of conformation is weighted sum over all states. Of cours magnetization is always equals 0, so we use magnetization squared.

$$m = \sum_i \sigma_i \qquad \langle m^2 \rangle = \frac{1}{Z} \sum_{\{\sigma\}} e^{-H\beta} m^2$$

We calculate magnetisation of Ising model using Wolf algorithm with cluster update. Then we average the values over all conformations.

Transition point

To determine the transition point in globules we tried to calculate Binder cumulant for sets of conformations with length of 250, 500, 1000, 2000, generated at low temperatures. Binder cumulant is calculated using this formula

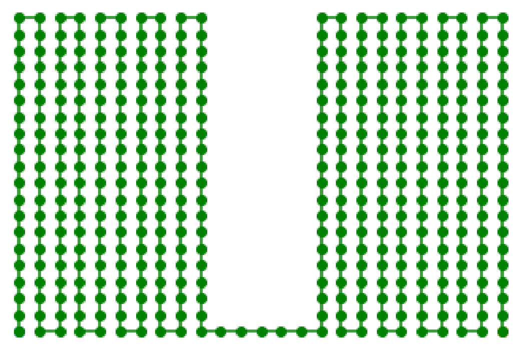
$$U = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}$$

The intersection point of the cumulants must be the transition point. But it appeared that not all conformations that are generated at low temperatures actually magnetic. Because of that high variance of magnetization from conformation to conformation we could not use Binder cumulant right away to determine the transition point.

Separation of conformations

To make the results clearer we decided to separate nonmagnetic conformations from generated sets. Looking at generated conformations we have noticed that nonemagnetic conformations can be represented as clusters of dencely placed vertexes and one-dimentional bridges which connect these clusters. At low temperatures, clusters are magnetized independently of each other and the probability that spins in them will have the opposite direction is close to 1/2. Because of that magnetization of conformation becomes significantly lower.

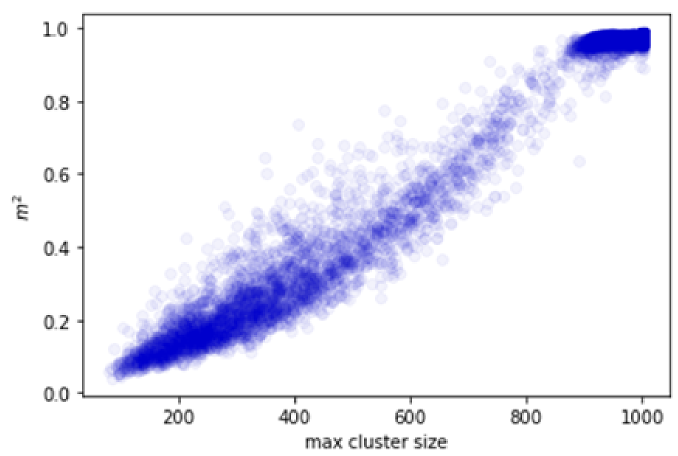
example of clusters and bridges in conformation



artificial example of conformation with 2 clusters

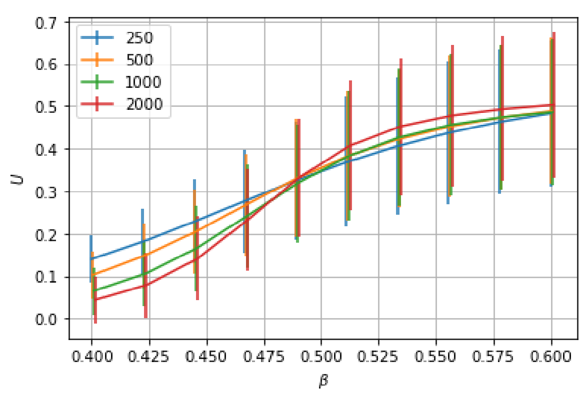
We have made an algorithm for determining clusters and bridges in conformations. It marks as clusters connected subgraphs in which all vertices have more than 2 neighbors. Bridges are connected subgraphs in which all vertices have 2 or 1 neighbor. And if both ends of the bridge are connected to the same cluster, then we do not consider it structurally significant since it does not separate clusters, so we consider it part of the cluster to which it is attached.

We chose the size of the largest cluster as the parameter by which we will separate the conformations on magnetic and nonemagnetic. Because at low temperatures the relationship between magnetization and the size of the largest cluster is almost linear and this parameter scales well with conformation length.

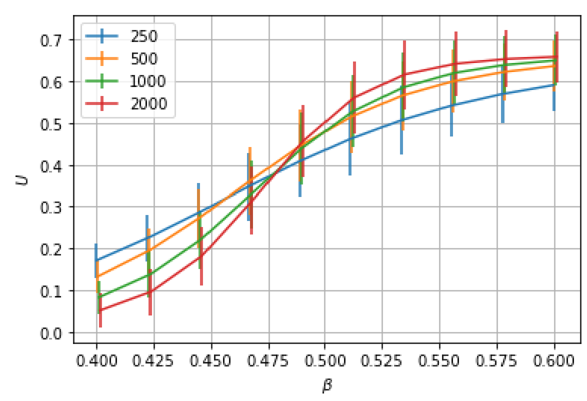


values of the squared magnetization and the size of the largest cluster for conformations of length 1000 at beta = 1

Using this method of separation appears to be effective, as it reduced variance of the cumulant in half. But it is still to big to accurately determine the transition point.



Cumulant on all generated conformations



Cumulant after separating magnetic conformations

Conclusion

- We can see that magnetization is directly related to the structure of magnetic domains in the conformation.
- Clusters size can be effectively used to determine magnetization of conformation.
- Separation of nonmagnetic conformations from generated set currently is not enough to determine the transition point. Results sugest that we should use something other than binder cumulant to detirmine transition point.