

Graph Theory and Statistical Physics

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Graph theoretical methods are used in studying statistical physics. The objective is to try to understand the graph theoretical phenomenon that appears in the critical region of the Ising model.

The Ising model was introduced in 1920 by Wilhelm Lenz as a model for ferromagnetism, and later studied by Ernst Ising. Ising could only solve it in one dimension; it took until 1944 before it was solved in the 2-dimensional case, without an external magnetic field, by Lars Onsager. The Ising model is perhaps the most studied model in statistical physics. Between 1969 and 1996 thousands of publications on this model have appeared.

The project started under the claim that the mathematical language of graph theory could be used to advance the study of spin models used in statistical physics. Our approach is to find scalable relations for the coefficients of the Ising partition function for graph families of interest in statistical physics, e.g., the cubic lattice. This is done by exact calculations of partition functions with external fields for small graphs and by Monte Carlo simulations of our own design for larger graphs.

There are also some previously unconsidered questions, inspired by the use of the model as an invariant for graphs, which are of interest from both a mathematical and physical point of view. Other work focuses on the Potts model and its connection to coloring of graphs.

Despite their simplicity, and hence some of their importance, both the Ising and Potts models generate highly complex behavior and in many cases one has to use computers to get to the relevant results. Within this field the project has produced additional ways of doing Monte Carlo approximation of the model for finite graphs. Among other things the method allows quite strong tests against computational errors, arising both from programming and from the method itself.

We have also used some of the methods from classical combinatorics in conjunction with new methods developed in Umeå to compute the partition function, the cornerstone of the model, for large finite graphs and we have extended these computations, using the HPC2N facilities, far beyond previous work. Other directions of work have applied similar methods to graph coloring, the Potts model as well as some other problems in matching theory, enumeration of independent sets and hardcore lattice gases.

For a graph G on n vertices and m edges, the Ising partition function is defined as

$$Z(G; x, y) = \sum_{i,j} a_{ij} x^i y^j$$

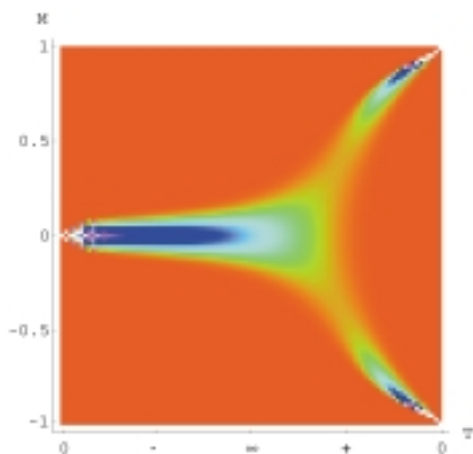
where a_{ij} is the number of bipartitions of the vertices into parts of order $(n-j)/2$ and $(n+j)/2$, respectively, with $(m-i)/2$ edges between them. To obtain the classical partition function it is then a matter of evaluating Z in the right point, i.e.,

$$Z(G; e^{-\beta J}, e^{-\beta H})$$

where $\beta = 1/(k_B T)$ with k_B being the Boltzmann constant and T is the temperature. The constants J and H describe the interaction between nearest-neighbors and an external field, respectively.

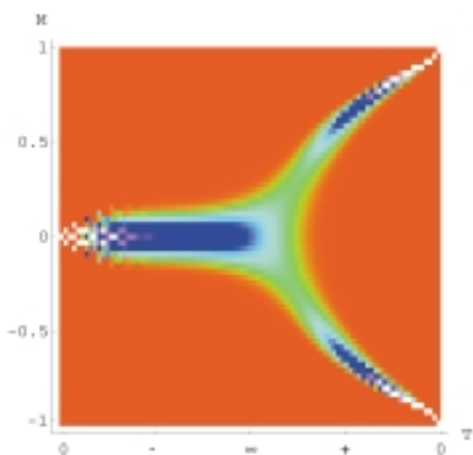
We have made extensive sampling of the Ising partition function on the 3-dimensional cubic lattice with cyclic boundary. Sampling the distribution of local energies (the total energy of the edges adjacent with a given vertex) gives us the possibility to reconstruct the derivative of the logarithm of the density-of-states function, which loosely speaking gives us a relation between temperature and energy. Moreover,

this distribution gives us a method-independent way of testing the correctness of our sampled data.



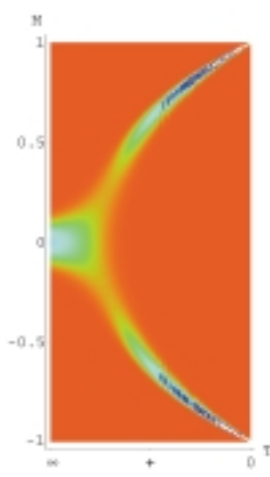
Plot showing the distribution of the magnetization, M , as function of the temperature, T , for the 10-by-10 lattice with cyclic boundaries $C_{10} \times C_{10}$. Red indicates regions with low probability, blue represents a high probability and white is a region with maximum probability. The broken symmetry at low temperatures is a characteristic feature of all ferromagnets.

We have reached the stage where we have enough information to give a good qualitative description of the scaling properties of the partition function in the whole range of possible coefficients. We are currently in the process of digesting these data. The programs can easily be adapted to make similar data sets for additional lattices of physical interest.

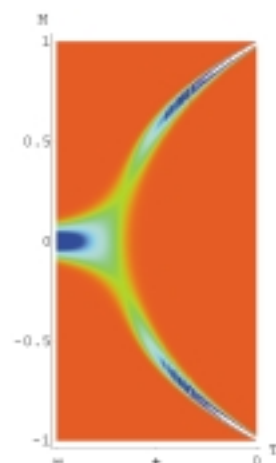


Plot showing the distribution of the magnetization, M , as function of the temperature, T , for the 4-by-4-by-4 lattice corresponding to the graph $C_4 \times C_4 \times C_4$.

We have also discovered some combinatorial properties of the partition function such as its connection with the matching polynomial and the independence polynomial. These polynomials have been heavily studied in statistical mechanics and theoretical chemistry.



Plot showing the distribution of the magnetization, M , as function of the temperature, T , for $C_6 \times C_6 \times C_6$ and $C_8 \times C_8 \times C_8$.



Further Readings

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