Statistical physics of graphs and networks – 2023-2024
Project: study of the configuration model of random graphs
Master in physics of complex systems

The purpose of this project is to study both the configuration model discussed during the lectures and a set of statistical mechanics problems defined on top of it.

The setting – Consider a graph with N vertices and assume that a fraction of them, $p_1 = 1 - \pi$, have degree 1 while the remaining fraction, $p_4 = \pi$, have a degree fixed to 4. The variable $\pi \in [0, 1]$ is a control parameter of the problems that follow.

Problem 1: Generation of instances of the random graph model.
Write a code and implement the algorithm to generate random instances of the configuration model described above. Implement the slightly biased version of the algorithm in which self-edges and multiple edges between pairs of nodes are rejected. Observe that the generated graphs are sparse and therefore think about a good data structure which allows an efficient representation of such graphs.

Problem 2: The giant component
The purpose of this problem is to study the emergence of a giant connected component.

(a) Generate random instances of the configuration model we are considering. For each instance, detect the largest connected component. Which algorithm do you use? Compute numerically the average size of the largest connected component and plot it for several values of π. What do you observe? What happens to these curves when increasing N? Note that the results become clearer when averaging them over several random graph instances.

(b) During the lectures, it was discussed a way to compute the giant connected component of random graphs extracted from $\mathcal{G}(N, c/N)$. Generalize this calculation to the configuration model considered here. Determine the critical value of π above which a giant connected component appears.

(c) Plot the theoretical prediction for the average size of the giant component against the result of the numerical simulations of point (a).

Problem 3: Emergence of the 3-core

(a) Generate random instances of the configuration model discussed here and compute numerically the size of the 3-core by implementing the algorithm discussed during the lectures. Plot the average size of the 3-core as a function of π for different values of N. Describe what you observe.

(b) Generalize the computation discussed during the lectures for the case $\mathcal{G}(N, c/N)$, to compute the average size of the 3-core of the configuration model that we are considering. Note that for this particular graph ensemble we have only a finite number of possible degrees and therefore the equations discussed in the lectures can be integrated numerically. Determine the critical value of π above which an extensive 3-core emerges. Is the transition continuous? What is the size of the 3-core for π just after the transition?

(c) Compare your theoretical predictions with the results of the simulations developed at the point (a).

Problem 4: The ferromagnetic Ising model
Consider the ferromagnetic Ising model described by the Hamiltonian

$$\begin{aligned} H &= -\sum_{\{i,j\} \in E:\ i<j} \sigma_i \sigma_j \\ \sigma_i &= \pm 1 \quad \forall i = 1, \ldots, N \end{aligned} \tag{1}$$

where the topology of the interactions is described by a random graph extracted from the configuration model we are considering here.

1. Simulate the model with a Monte Carlo Markov Chain (MCMC) for several temperatures T and several values of π. For each T and π measure the magnetization of the system defined as $m = \sum_{i=1}^{N} \sigma_i / N$ for several equilibrium configurations and plot the corresponding histogram. How can you detect the critical temperature of the ferromagnetic transition from this plot?
2. Implement the Belief Propagation (BP) equations on specific instances of the random graph model. Find the phase transition point and compare the results of BP with the MCMC simulations.
3. Compute the ensemble-averaged distribution of the cavity fields and of the effective fields using the population dynamics algorithm and determine the ensemble-averaged phase diagram by generalizing the computations discussed during the lectures to the random graph ensemble considered here.

Problem 5: Inverse Ising model

Extract a large number M of i.i.d. equilibrium samples $\{\sigma_i^{(m)}\}_{i=1,\ldots,N}^{m=1,\ldots,M}$ of the ferromagnetic Ising model discussed in the problem 4. Sample such configurations at a temperature above the critical one so that the configurations are typical of the paramagnetic phase. We want to reconstruct the underlying graph from such samples.

1. Compute numerically the connected correlations functions $C_{ij} = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$ from the samples and for all pairs $i < j$. Sort the pairs according to their correlation and determine the positive predictive value (number of true positive predicted edges/number of predictions) as a function of the number of predictions (strongest correlated pairs).
2. Use the mean-field approximation to infer the underlying graph.
3. Plot histograms for the estimated connected correlations and the inferred couplings, separated into the cases of pairs connected by an edge in the graph and unconnected pairs. Discuss what you observe.