Statistical physics of Graphs and Networks
Project: The Configuration Model of Random Graphs

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Objective of this project is the analysis of the configuration model for random graphs of given degree distribution. It follows the analysis given in the lectures for finite connectivity random graphs. To have a well defined setting, our graphs of N vertices have the simple degree distribution $p_1 = 1 - \pi, p_4 = \pi$, i.e., a fraction $\pi \in [0, 1]$ of vertices have degree four, the other vertices have degree one. Note that this graph consists of $N/2$ isolated dimers in the case $\pi = 0$, and it is a 4-regular graph for $\pi = 1$.

Problem 1: Generation of random graphs of given degree distribution
Implement the algorithm for generating graphs of given vertex number and vertex degree distribution. Use the (slightly biased) version of the algorithm presented in the lectures, which does not accept multiple edges and self-edges. Think about a good data structure (the graph is sparse!), which allows to efficiently address the following questions.

Problem 2: Emergence of the giant component
(a) Generalize the analytic calculation of the size of the giant component from random graphs in $\mathcal{G}(N, c/N)$ to the configuration model. Determine the critical value of π, at which the giant component emerges.
(b) Determine the size of the largest connected component numerically for individual graphs of different vertex numbers. Note that results become clearer, when you average over several realisations of the random graph, and when you go to larger values of N.
(c) Plot the results of (a) and (b) in a single figure. Discuss finite size effects.

Problem 3: Emergence of the 3-core
(a) Generalise the analytical calculation for the dynamics of the 3-core algorithm from $\mathcal{G}(N, c/N)$ to our graph ensemble – note that due to the finite number of possible degrees, these equation can easily be solved numerically, whereas an ansatz similar to the lectures is difficult. Determine the critical threshold π for the emergence of the 3-core. Is the transition continuous or not? What is the size of the 3-core just after the transition?
(b) Compare the analytical results of (a) with those of a direct implementation of the 3-core algorithm for specific graph instances.

Problem 4: The ferromagnatic Ising model
The ferromagnetic Ising model is given by its Hamiltonian

$$\mathcal{H} = - \sum_{\{i,j\} \in E} S_i S_j$$

for N Ising spins $S_i = \pm 1, i = 1, ..., N$.
(a) Simulate the Ising model (MCMC), and determine, for several temperatures and several values of π, the histograms of the global magnetisation $M = \frac{1}{N} \sum_i S_i$ over many equilibrium configurations of the model. How can you find the phase transition temperature T_c from this histogram?
(b) Implement the equations of belief propagation (BP) on specific instances of the random graph. Find the phase transiton temperature, and compare the results of BP with the MC simulations.
(c) Determine the ensemble-averaged distribution of effective fields using the population-dynamics algorithm, and the corresponding ensemble-averaged phase diagram, generalising the analytical calculations done in the lectures for random graphs.

Problem 5: Inverse Ising model and graph reconstruction
Use a large i.i.d. sample $\{S_i^m\}_{i=1,..,N}^{m=1,...,M}$ of configurations sampled from the Ising model in the paramagnatic phase, to reconstruct the underlying graph.
(a) Estimate the connected correlations $c_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$ from the sample, for all pairs $1 \leq i < j \leq N$. Sort the pairs according to their correlation, and determine the positive predictive value (number of true postive predicted edges / number of predictions) as a function of the number of predictions (strongest correlated pairs).
(b) Use the mean-field approximation to infer the underlying graph.
(c) 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. What do you observe?