Large-deviation properties of largest 2-core component for random graphs

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Abstract. Distributions of the size of the largest component of the 2-core for Erdős-Rényi (ER) random graphs with finite connectivity c and a finite number N of nodes are studied. The distributions are obtained basically over the full range of the support, with probabilities down to value as small as 10^{-320}. This is achieved by using an artificial finite-temperature (Boltzmann) ensemble. The distributions for the 2-core resemble roughly the results obtained previously for the largest components of the full ER random graphs, but they are shifted to much smaller probabilities ($c \leq 1$) or to smaller sizes ($c > 1$). The numerical data is compatible with a convergence of the rate function to a limiting shape, i.e., the large-deviations principle apparently holds.

1 Introduction

The result of any random process can be represented by a probability distribution or by a probability density. Only for few cases analytical results can be obtained. Thus, most problems have to be studied by numerical simulations [1], in particular by Monte Carlo (MC) techniques [2,3]. In numerical work, one often addresses only the *typical* region of such a distribution, where the probabilities (or densities) are large, say in the range $[10^{-6}, 1]$. Nevertheless, for many problems in science and in statistics, one would like to obtain (almost) the full distribution, i.e., the large deviation properties play an important role [4,5]. For the present work, we are interested in sampling and evaluating a set ob random objects. There are many examples in sciences, e.g, one samples graphs, disordered magnets, protein sequences, or finite-dimensional paths. This is usually called *quenched average*. Classically, sampling the quenched averaged has been performed via a finite set of independently drawn instances. Some years ago it has been noted that by introducing an artificial sampling temperature the large-deviation properties with respect to the quenched random ensemble can be obtained [6]. This corresponds somehow to an annealed average (where the randomness fluctuates together with the dynamic degrees often defined on top of the random objects), but the results are re-weighted in a way that the results for the original quenched ensemble are obtained. In this way, the large-deviation properties of the distribution of alignment scores for protein comparison was studied [6–8], which is of importance to calculate the significance of results of protein-data-base queries [9].

Motivated by these results, similar approaches have been applied to other problems like the distribution of the number of components of Erdős-Rényi (ER) random

graphs [10], the partition function of Potts models [11], the distribution of ground-state energies of spin glasses [12] and of directed polymers in random media [13], the distribution of Lee-Yang zeros for spin glasses [14], the distribution of success probabilities of error-correcting codes [15], the distribution of free energies of RNA secondary structures [16], some large-deviation properties of random matrices [17,18], the distribution of endpoints of fractional Brownian motion with absorbing boundaries [19], and the distribution of work performed by an Ising system [20].

For the case of the distribution of the size of the larges component of the ER random graphs [21], also a comparison to exact analytical results was performed. For small connectivities $c < 1$, i.e., below the percolation threshold, even for moderate system sizes, a very good agreement between analytical and numerical results was found, for the full range of the support, even in the range of very small probabilities like 10^{-160}. Beyond the percolation threshold $c > 1$ stronger finite size effects were observed, but a convergence towards the analytical solution was visible.

In the present work, the same approach is applied to the related problem of analysing the distribution of the size of the largest component of the 2-core. The q-core is the sub graph which is remaining after iteratively removing all nodes which have a degree less than q, including removing the incident edges. For this case no analytical solution is known to the author. In the present work these results are shown for $q = 2$ togther with the result for the largest component of the full graph to highlight similaryties and differences. Additionally, for the case of the larges component for $c > 1$ the comparison to the analytical result is updated, since there was a mistake in Ref. [21].

To fix notations, a *graph* $G = (V, E)$ consists of N nodes $i \in V$ and undirected edges $\{i, j\} \in E \subset V^{(2)}$. For each edge $\{i, j\} \in E$ the nodes i and j are called *adjacent*. The edge is called *incident* to its two nodes. The *degree* of a node $i \in V$ is the number of adjacent nodes. A *subgraph* G' of G is a graph $G' = (V', E')$ with $V' \subset V$ and $E' \subset E$. The *q-core* of a graph is the subgraph which is remaining after iteratively removing all nodes with degree smaller than q, and removing the edges incidents to these nodes. Thus, for the q-core all nodes have degree at least q. Here, we concentrate on the case $q = 2$. Two nodes i, j are called *connected* if there exist a *path* of disjoint edges $\{i_0, i_1\}, \{i_1, i_2\}, \ldots, \{i_{l-1}, i_l\}$ such that $i = i_0$ and $j = i_l$. The maximum-size subsets $C \subset V$ of nodes, such that all pairs $i, j \in C$ are connected are called the (connected) *components* of a graph. The size of the largest component of a graph, or of the largest component of the corresponding 2-core, is denoted here by S.

Here, we do not study graphs occuring in the real world, but random graphs, which can be generated by algorithms in the computer. ER random graphs [22] have N nodes and each possible edge $\{i, j\}$ is present with probability c/N. Hence, the average degree (connectivity) is c.

Via the random-graph enembles, a probability distribution $P(S)$ for the size of the largest component and the corresponding probability $P(s)$ for relative sizes $s = S/N$ are defined. The probabilities $P(s)$ for values of s different from the typical size are exponentiall small in N. Hence, one uses the concept of the large-deviation *rate function* [4] by writing

$$P(s) = e^{-N\Phi(s) + o(N)} \quad (N \to \infty) \tag{1}$$

This leading-order behavior of the large-deviation rate function $\Phi_{\mathrm{ER}}(s, c)$ for ER random graphs with connectivity c is known exactly [23] and given by the following set of equations for $s \in [0, 1]$. For $c > 1$ the rate function is defined piecewise on several intervals $[s_k, s_{k-1}]$:

$$s_0 = 1$$
$$s_k = \sup\left\{s : \frac{s}{1-ks} = 1 - e^{-cs}\right\}$$
$$m(y) = \log(1 - e^{-y})$$
$$\Phi_{\mathrm{ER}}(s,c) = -ksm(cs) + ks\log s + (1-ks)\log(1-ks) + cks - k(k+1)cs^2/2$$
$$\text{for} s_k < s \leq s_{k-1}. \tag{2}$$

Note that for $c \leq 1$ we have $s_1 = 0$, i.e. only the case $k = 0$ is relevant. Note also that in Ref. [23] there is a small misprint which states for the forth term of $\Phi_{\mathrm{ER}}(s,c)$ cs instead of the correct cks.

For the case of the largest component of the 2-core, no analytical result is known to the author.

The paper is organised as follows. In the second section, the numerical simulation technique and the corresponding re-weighting approach are explained. In the third section, the results are displayed for the 2-core of the ER random graph ensemble, in comparison to the results for the largest component of the orignal graph, as obtained before. Finally, a summary and an outlook are given.

2 Simulation and reweighting method

We are interested in determining the distribution $P(S)$ for any measurable quantity S. Here S is the largest component of a graph or of the 2-core of a graph. The distribution is over any graph ensemble, here the ER random graphs. *Simple sampling* is straightforward: One generates a certain number K of graph samples and obtains $S(G)$ for each sample G. This means each graph G will appear with its natural ensemble probability $Q(G)$. The probability to measure a value of S is given by

$$P(S) = \sum_G Q(G)\delta_{S(G),S} \tag{3}$$

Therefore, by calculating a histogram of the values for S, a good estimation for $P(S)$ is obtained. Nevertheless, $P(S)$ can only be measured in a regime where $P(S)$ is relatively large, about $P(S) > 1/K$. Unfortunately, the distribution decreases exponentially fast in the system size N when moving away from its typical (peak) value. This means, even for moderate system sizes N, the distribution will be unknown on almost its complete support.

To estimate $P(S)$ for a much larger range, even possibly on the full support of $P(S)$, where probabilities smaller than, e.g., 10^{-300} may appear, a different approach is used [6,21]. For self-containedness, the method is outlined subsequently. The basic idea is to use an additional Boltzmann factor $\exp(-S(G)/T)$, T being a "temperature" parameter, in the following manner: A standard Markov-chain MC simulation [2,3] is performed, where the current state at "time" t is given by an instance of a graph $G(t)$. Here the Metropolis-Hasting algorithm is applied [24]. In in each step t from the current graph $G(t)$ a *candidate* graph G^* is created. Here, a local update is used which works in the following way: A node i of the current graph is selected randomly, with uniform weight $1/N$, and all adjacent edges are deleted. For all feasible edges $\{i, j\}$, the edge is added with a weight corresponding to the natural weight $Q(G)$, i.e., with probability c/N for the ER random graph. For the candidate graph, the size of the largest component is calculated, or the size of the largest component of

the 2-core, depending on what we are interested to measure. This size is denoted as $S(G^*)$. Finally, the candidate graph is *accepted*, $(G(t+1) = G^*)$ with the Metropolis probability

$$p_{\mathrm{Met}} = \min \left\{ 1, e^{-[S(G^*)-S(G(t))]/T} \right\} . \qquad (4)$$

Otherwise the current graph is kept $(G(t+1) = G(t))$. By construction, the algorithm fulfills detailed balance. Clearly the algorithm is also ergodic, since within N steps, each possible graph may be constructed. Thus, in the limit of infinite long Markov chains, the distribution of graphs will follow the probability

$$q_T(G) = \frac{1}{Z(T)} Q(G) e^{-S(G)/T} , \qquad (5)$$

where $Z(T)$ is the a priori unknown normalisation factor.

The distribution for S at temperature T is given by

$$P_T(S) = \sum_G q_T(G)\delta_{S(G),S}$$

$$\overset{(5)}{=} \frac{1}{Z(T)} \sum_G Q(G) e^{-S(G)/T} \delta_{S(G),S}$$

$$= \frac{e^{-S/T}}{Z(T)} \sum_G Q(G)\delta_{S(G),S}$$

$$\overset{(3)}{=} \frac{e^{-S/T}}{Z(T)} P(S)$$

$$\Rightarrow \quad P(S) = e^{S/T} Z(T) P_T(S) \qquad (6)$$

Hence, the target distribution $P(S)$ can be estimated, up to a normalisation constant $Z(T)$, from sampling at finite temperature T. For each temperature, a specific range of the distribution $P(S)$ will be sampled: Using a positive temperature allows to sample the region of a distribution left to its peak (values smaller than the typical value). Since T is only an artificial resampling parameter, also negative temperatures are feasible, which allow us to access the right tail of $P(S)$. Temperatures of large absolute value will cause a sampling of the distribution close to its typical value, while temperatures of small absolute value are used to access the tails of the distribution. Hence one chooses a suitable set of temperatures $\{T_{-N_n}, T_{-N_n+1}, \ldots, T_{N_p-1}, T_{N_p}\}$ iteratively (see below), N_n and N_p being the number of negative and positive temperatures, respectively. Via obtaining the distributions $P_{T_{-N_n}}(S), \ldots, P_{T_{N_p}}(S)$, such that $P(S)$ is "covered" as much as possible, one can measure $P(S)$ over a large range, possibly on its full support.

The normalisation constants $Z(T)$ can easily be obtained by including a histogram obtained from simple sampling, which corresponds to temperature $T = \pm\infty$, which means $Z \approx 1$ (within numerical accuracy). Using suitably chosen temperatures T_{+1}, T_{-1}, one measures histograms which overlap with the simple sampling histogram on its left and right border, respectively. Then the corresponding normalisation constants $Z(T_{\pm 1})$ can be obtained by the requirement that after rescaling the histograms according to (6), they must agree in the overlapping regions with the simple sampling histogram within error bars. This means, the histograms are "glued" together. In the same manner, the range of covered S values can be extended iteratively to the left and to the right by choosing additional suitable temperatures $T_{\pm 2}, T_{\pm 3}, \ldots$ and glueing the resulting histograms one to the other. A pedagogical explanation and examples of this procedure can be found in Ref. [25].
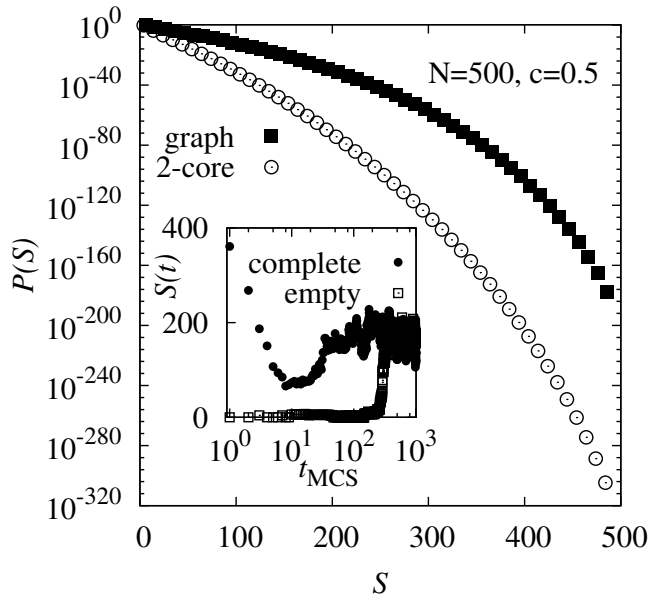
Fig. 1. Distribution of the size S of the largest component ("graph") and of the largest component of the 2-core for Erdős-Rényi random graphs of size $N = 500$ at connectivity $c = 0.5$. In this and all other plots, error bars are of symbol size or smaller if not explicitly shown. Note that the data was obtained for actually for all 500 (or 501) possible values of S, here the data is thinned out (not averaged!) for clarity. The inset shows the size of the largest 2-core as function of the number t_{MCS} of Monte Carlo sweeps for the same type of graphs at temperature $T = -1$. Two different starting conditions are displayed: either an empty graph ($S = 0$) or a complete graph ($S = 500$) was used.

In order to obtain the correct result, the MC simulations must be equilibrated. For the case of the distribution of the size of the largest component, this is very easy to verify: The equilibration of the simulation can be monitored by starting with two different initial graphs $G(t = 0)$, respectively:

– Either an empty graph is taken, i.e., it has N nodes but no edges. This means that the largest component is of size one, the 2-core is empty. In the inset of Fig. 1 the evolution of the size S of the largest component of the 2-core as a function of the number $t_{MCS} = t/N$ of Monte Carlo sweeps is shown for Erdős-Rény random graphs with $N = 500$ nodes, connectivity $c = 0.5$ at temperature $T = -1$. As $c > 0$ edges will be added to the initial empty graph during the Markov-chain Monte Carlo simulation. As one can see, $S(t_{MCS})$ moves after some initial equilibration time away from zero towards a values around $S = 150$.
– Alternatively one can start with a complete graph, which contains all $N(N-1)/2$ possible edges. For this graph the largest component contains all N nodes, also for the 2-core. Here $S(t_{MCS})$ starts on the opposite side of the possible values, i.e., $S(t_{MCS} = 0) = N$. During the Monte Carlo evolution, since $c \ll N$, the graph will evolve on average towards having less edges, resulting in a decrease of $S(t_{MCS})$.

In any case, for the two different initial conditions, the evolution of $S(t_{MCS})$ will approach from two different extremes, which allows for a simple equilibration test: equilibration is achieved if the measured values of S agree within the range of fluctuations. Only data was used in this work, where equilibration was achieved with less than 1000 Monte Carlo sweeps.

The resulting distribution for ER random graphs ($c = 0.5$, $N = 500$) is shown in the main plot of Fig. 1. As one can see, the distribution can be measured over its full support such that probabilities as small as 10^{-160} for the largest compoents and even 10^{-320} for the largest component of the 2-core are accessible.

Note that in principle one can also use a Wang-Landau approach [26] or similar approaches to obtain the distribution $P(S)$ without the need to perform independent simulations at different values for the temperatures. Nevertheless, the author has performed tests for ER random graphs and experienced problems by using the Wang-Landau approach, because the sampled distributions tend to stay in a limited fraction of the values of interest. Using the finite-temperature approach it is much easier to guide the simulations to the regions of interest, e.g., where data is missing using the so-far-obtained data, and to monitor the equilibration process.

3 Results

ER random graphs of size up $N = 500$ were studied. In few cases, additional system sizes ($N = 50, 100, 200$) were considered to estimate the strength of finite-size effects, see below. For ER random graphs there exists a percolation transition marked by the appearence of a largest component of order of system size (called "giant component") at $c = c_{\rm c} \equiv 1$. At the same point there is a percolation transition for the 2-core [27], see also the pedagogical presentation in Ref. [28]. Since the percolation transition of the graph and of the 2-core are the same vaue of the connectivity, the results for $P(S)$ can be conveniently compared. The model was studied right at the percolation transition, for one point in the non-percolating regime ($c = 0.5$) , and for one point in the percolating regime ($c = 2$). The temperature ranges used for the different cases are shown in Tab. 1. Note that for each quanity S of interest a separate set of simulations has to be peformed, since the reweighting is done with the corresponding value S (the simulations for the largest component of the full graph were performed in the project leading to the publication of Ref. [21].) This means also that the sets of temperatures actually differ for measuring the size of the largest component of the full graph and for measuring the size of the largest component of the 2-core. Note furthermore that, depending on the position of the peak of the size distribution, sometimes only negative and sometimes negative as well as positive temperatures had to be used.

For the systems listed in the table, the length of the MC simulation was 10^5 sweeps, to have a high-quality statistics. Equilibration was always achieved within the first 1000 MCS, thus the graphs from these initial parts of the simulations were excluded from the analysis. In general, studying significantly larger sizes or going deeper into the percolation regime makes the equilibration much more difficult.

For the case of the largest component of ER random graphs the analytical result (2) can be used for comparison [21]. This allows to assess the quality of the method and to get an impression of influence of the non-leading finite-size corrections.

In Fig. 2 the empirical rate function

$$\Phi(s) \equiv -\frac{1}{N} \log P(s) \tag{7}$$

for $c = 0.5$ is displayed, corresponding to the distribution shown in Fig. 1. Note that by just stating the analytical asymptotic rate function $\Phi_{\rm ER}(s, c)$, the corresponding distribution $P(s)$ is not normalised. Hence, for comparison, $\Phi(s)$ is shifted for all values of the connectivity c such that it is zero at its minimum value, like $\Phi_{\rm ER}(s, c)$.

The numerical data for the size of the largest component of the graph agrees very well with the analytic result. Only in the region of intermediate cluster sizes, a

system	$T_{\min}$	$T_{\max}$	N_T
full ER $c = 0.5$	-5	-0.4	14
full ER $c = 1.0$	-7.0	-0.6	9
full ER $c = 2.0$	-2.0	10.0	6
2-core ER $c = 0.5$	-150	-0.2	14
2-core ER $c = 1.0$	-10.0	-0.2	15
2-core ER $c = 2.0$	-10.0	5.0	16

Table 1. Parameters used to determine the distributions $P(S)$ for the different models. $T_{\min}$ is the minimum and $T_{\max}$ the maximum temperature used. Also always included was a histogram from simple sampling, corresponding to $T = \infty$. N_T denotes the total number of different temperature values ($N = 500$). For smaller sizes a somehow smaller number of temperatures is needed.
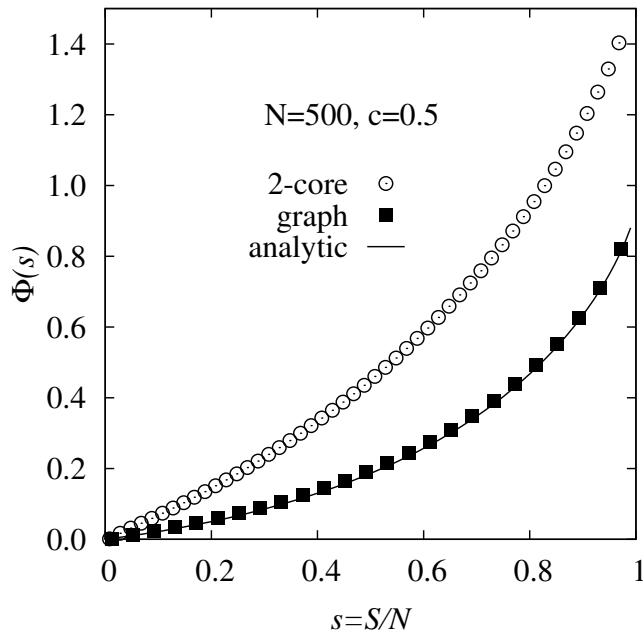
Fig. 2. Large-deviation rate function $\Phi(s)$ for the relative 2-core size s of ER random graphs with average connectivity $c = 0.5 < c_c$, $N = 500$ (circle symbols). For comparison the results for the rate function of the relative size s of the larges component is included. The line displays the analytical result for the largest component as shown in Eq. (2).

small systematic deviation is visible, which is likely to be a finite-size effect. Given that for the numerical simulations only graphs with $N = 500$ nodes were treated, the agreement with the $N \to \infty$ leading-order analytical result is remarkable. Thus, we can assume, that at least in this region of configuration space, small graphs are sufficiently close to the $N \to \infty$ limiting behavior. The distribution of the size of the largest component of the 2-core looks very similar, but exhibits larger values, corresponding to much smaller probabilities. This is natural, since for almost each graph its largest component of the 2-core is smaller than the largest component of the graph. Note that the shape of the distributions look rather similar. But a simple rescaling of the y-axis does not allow for a collaps of the data, which shows that the shapes are actually very different.
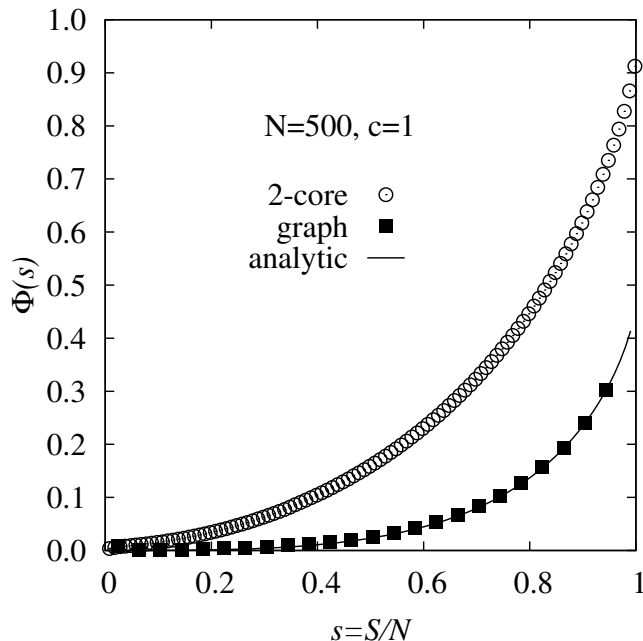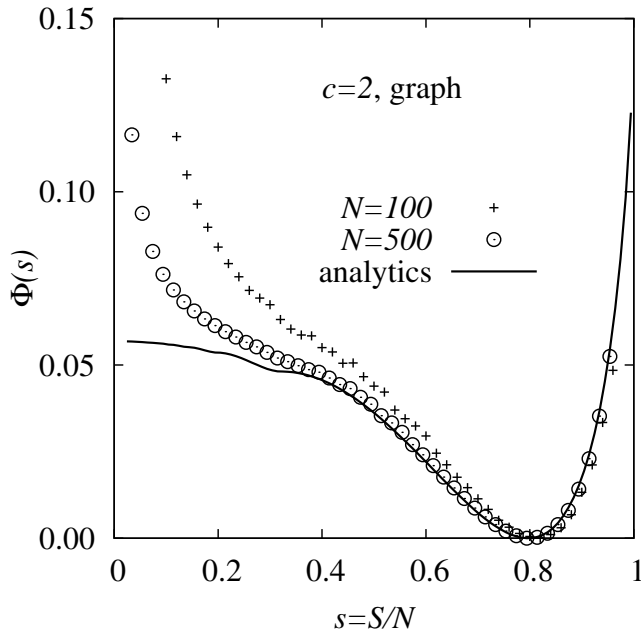
Fig. 3. Large-deviation rate function $\Phi(s)$ for the relative 2-core size s of ER random graphs with average connectivity $c = 1 = c_{\text{c}}$, $N = 500$ (circle symbols). For comparison the results for the rate function of the relative size s of the larges component is included. The line displays the analytical result for the largest component as shown in Eq. (2).

The resulting rate function right at the percolation transition $c = c_{\text{c}} = 1$ is shown in Fig. 3. Qualitatively, the results are very similar to the non-percolating case $c = 0.5$, except that the distributions are much broader, corresponding to smaller values of the rate function. Again, the agreement with the analytical result for the largest component of the graph is very good, which also indicates a weak finite-size effect. This indicates that also the result for the 2-core might be actually already close to the large-graph limit. Like for $c = 0.5$, the corresponding rate function values for the 2-core are above the values for the full graphs, whith the same explenation.

The case of the percolating regime (connectivity $c = 2$), is displayed for the largest component of the full graph in Fig. 4. The rate function exhibits a minimum at a finite value of s, corresponding to the finite average fraction of nodes contained in the largest component. Note that the numerical data was already published in Ref. [21], but there the analytical result was slightly incorrect. For this reason, the data is shown here again together with the correct rate function. For most of the support of the distribution, the numerical data for $N = 500$ agrees again very well with the analytic result. Nevertheless, for $s \to 0$, strong deviations become visible because the numerical rate function $\Phi(s)$ grows strongly as $s \to 0$. In comparison to $c \leq 1$, strong finite-size deviations are visible.

In Fig. 5 the rate function for the largest component of the 2-core is shown. The rate function also exhibits a minimum, corresponding to the typical size of the largest component. This minimum is shifted to the left as compared to the case of the full graph. Also large sizes are much less likely for the 2-core case. This appears, again, to be natural because for sparse graphs the largest component of the 2-core is basically always smaller than the largest component of the full graph. Here no analytic results are available. Nevertheless, the finite-size dependence of the result appears to be very weak, which indicates that the limiting rate function will look very similar. Note that

Fig. 4. Large-deviation rate function $\Phi(s)$ for the size of the largest component of ER random graphs with average connectivity $c = 2 > c_{\mathrm{c}}$, $N = 100$ and $N = 500$ (symbols). The line displays the analytical result from Eq. (2).

actually the strongest finite-size effect is not visible here, since it was removed by a shift of the function such that at the minimum $\Phi(s_{\min}) = 0$. This shift deacreses from 0.0575 for $N = 50$ to 0.0079 for $N = 500$, indicating that for $N \to \infty$ no shift is needed. In particular, there seems also here to exist a limiting rate function, meaning that the large-deviation principle holds.

4 Summary and outlook

By using an artificial Boltzmann ensemble characterised by an artificial temperature T, the distributions of the size of the largest component and of the largest component of the 2-core for ER randoms graphs with finite connectivity c have been studied in this work. For not too large system sizes, the distributions can be calculated numerically over the full support, giving access to very small probabilities such as 10^{-320}.

For the ER case, the numerical results for the large-deviation rate function $\Phi(s)$, obtained for rather small graphs of size $N = 500$, agree very well with analytical results obtained previously for the leading behaviour in the limit $N \to \infty$. This proves the usefulness of the numerical approach, which has been applied previously to models where no complete comparison between numerical data and exact analytic results have been performed. Note that the results for the case of the full graphs have been published before [21] and are included here mainly for comparison. Nevertheless, the analytic result stated in Ref. [21] for $c > 1$ was slightly incorrect, while here now the correct analytical rate function is given.

The main findings are that below and at the percolation transition, $\Phi(s)$ exhibits a minimum at $s = 0$ and rises monotonously for $s \to 1$. This holds for the full graph as well as for the 2-core case. Only, for each component-size S, the corresponding probability is (much) smaller for the 2-core case as compared to the full graph. Inside
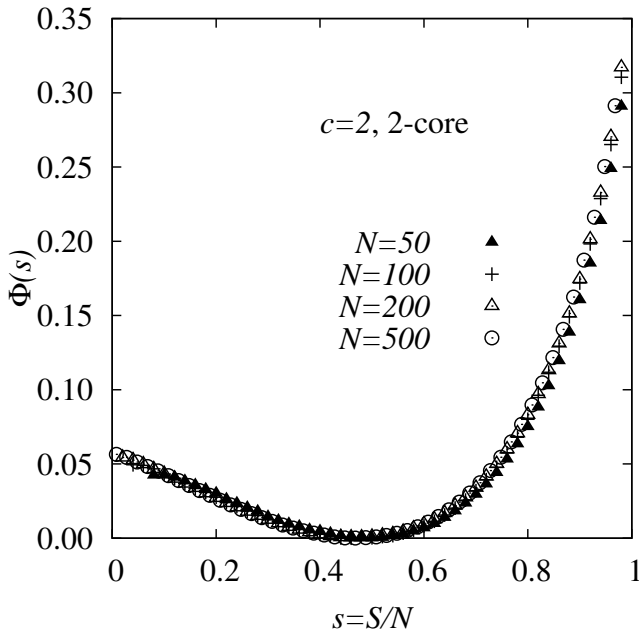
Fig. 5. Large-deviation rate function $\Phi(s)$ for the relative size of the largest 2-core of ER random graphs with average connectivity $c = 2 > c_c$, $N = 50$, $N = 100$, $N = 200$ and $N = 500$. A convergence to a limiting rate functions appears to be compatible with the data.

the percolating regime, $\Phi(s)$ exhibits a minimum, grows quickly around this minimum and levels off horizontally for $s \to 0$. The rate function for the 2-core case is shifted to the left, again due to smaller sizes of the 2-core for spares graphs

The finite-size corrections are usually small, except for the largest component of the full graph in percolating regime ($c > 1$) in an extended region near $s = 0$. Interestingly, for the 2-core case, the finite-size corrections concerning the shape of the rate function appear to be always small.

Since the comparison with the exact results for the ER random graphs indicates the usefulness of this approach to study large-deviation properties of random graphs, it appears promising to consider many other properties of different ensembles of random graphs in the same way. For example, it would be interesting to obtain the distribution of the diameter of ER random graphs, where only for $c < 1$ there is an analytic result available. Corresponding simulations are currently performed by the author of this work.

Note that with respect to the q-core, here we have focused on the 2-core, which exhibits a second order phase transition at $c = 1$. For the 3-core this shifts to $c \approx 3.35$ and becomes first order (see also the numerical results in Ref. [28]). The distributions fall off in same regions extremely quickly (with, e.g., a factor of 10^{-9} between two adjacent values of S), as tests performed by the author show. This makes it much harder for addressing the distributions over the full range of support even when using sophisticated large-deviations approaches.

Acknowledgements

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