Rare events statistics of random walks on networks: localisation and other dynamical phase transitions

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Abstract. Rare event statistics for random walks on complex networks are investigated using the large deviation formalism. Within this formalism, rare events are realised as typical events in a suitably deformed path-ensemble, and their statistics can be studied in terms of spectral properties of a deformed Markov transition matrix. We observe two different types of phase transition in such systems: (i) rare events which are singled out for sufficiently large values of the deformation parameter may correspond to *localised* modes of the deformed transition matrix; (ii) "mode-switching transitions" may occur as the deformation parameter is varied. Details depend on the nature of the observable for which the rare event statistics is studied, as well as on the underlying graph ensemble. In the present paper we report results on rare events statistics for path averages of random walks in Erdős-Rényi and scale free networks. Large deviation rate functions and localisation properties are studied numerically. For observables of the type considered here, we also derive an analytical approximation for the Legendre transform of the large deviation rate function, which is valid in the large connectivity limit. It is found to agree well with simulations.

1. Introduction

Random walks are dynamical processes widely used to analyse, organise or perform important tasks on networks such as searches [1, 2], routing or data transport [3, 4, 5]. Their popularity is due to their cheap implementability, as they rely only on local information, such as the state of the neighbourhood of a given node of the network. This ensures network scalability and allows fast data transmission without the need for large storage facilities at nodes, such as big routing tables in communication networks. These features make random walks an efficient tool to explore networks characterised by a high cost of information. Examples are sensor networks [6] where many signalling packets are needed to acquire wider networks status information. In peer-to-peer networks the absence of a central server storing file locations requires users to perform repeated local searches in order to find a file to download, and various random walk strategies have been proposed as a scalable method [7, 8, 9] in this context. Less attention has been paid to characterise rare events associated with random walks on networks. Yet the occurrence of a rare event can have severe consequences. In hide-and-seek games, for instance [10], rare events represent situations where the seeker finds either most (or unusually many) of the hidden targets, or conversely none (or unusually few). In the context of cyber-security, where one is concerned with worms and viruses performing random walks through a network, a rare event would correspond to a situation where unusually many sensitive nodes are successfully attacked and infected, which may have catastrophic consequences for the integrity of an entire IT infrastructure. Characterising the statistics of rare events for random walks in complex networks and its dependence on network topology is thus a problem of considerable technological importance. A variant of this problem was recently analysed for biased random walks in complex networks [11]. That paper addressed rare fluctuations in single node occupancy for an ensemble of independent (biased) walkers in the stationary state of the system. By contrast, our interest here is in rare event statistics of *path averages*, or equivalently of time integrated variables. Rare event statistics of this type has been looked at for instance in the context of kinetically constrained models of glassy relaxation [12]; relations to constrained ensembles of trajectories were explored in [13] for Glauber dynamics in the 1d Ising chain. While these studies were primarily concerned with the use of large deviation theory as a tool to explore dynamical phase transitions in homogeneous systems, our focus here is on the interplay between rare event statistics and the heterogeneity of the underlying system.

In the present paper we use large deviation theory to study rare events statistics for path averages of observables associated with sites visited along trajectories of random walks. Within this formalism, rare events are realised as typical events in a suitably deformed path-ensemble [14, 12]. Their statistics can be studied in terms of spectral properties of a deformed version of the Markov transition matrix for the original random walk model, the relevant information being extracted from the algebraically largest eigenvalue of the deformed transition matrix. Such deformations may direct random walks to subsets of a network with vertices of either atypically high or atypically low degree. It also amplifies the heterogeneity of transition matrix elements for large values of the deformation parameter and we observe that, as a consequence, the eigenvector corresponding to the largest eigenvalue of the deformed transition matrix may exhibit a *localisation transition*, indicating that rare large fluctuations of path averages are typically realised by trajectories that remain localised on small subsets of the network. Within localised phases, we also encounter a second type of dynamical phase transition related to *switching between modes* as the deformation parameter used to select rare events is varied. Our methods allow us to study the role that network topology and heterogeneity play in selecting these special paths, as well as to infer properties of paths actually selected to realise extreme events. Given the variety of different path averages and graph ensembles one might consider, a complete exploration of the problem within the present paper is clearly out of the question. In what follows, we report results for Erdős-Rényi (ER) networks and for scale free (SF) networks obtained by a preferential attachment algorithm and we shall further restrict ourselves to two types of path average to be specified below.

2. The model

2.1. Setup of the problem

We consider a complex network with adjacency matrix A, with entries $a_{ij} = a_{ji} = 1$ if the edge (ij) exists, and $a_{ij} = 0$ otherwise. The transition matrix W of an unbiased random walk has entries $W_{ij} = a_{ij}/k_j$ where k_j is the degree of node j, i.e. $k_j = \sum_i a_{ij}$, and W_{ij} is the probability of a transition from j to i. While we restrict ourselves in the present paper to analyse rare-events for unbiased random walks, we remark at the outset that our method is not restricted to this case, and that more general hopping processes, including irreversible ones, can be studied by our approach.

Writing $\mathbf{i}_\ell = (i_0, i_1, \cdots, i_\ell)$ a path of length ℓ, quantities of interest are empirical path-averages of the form

$$\hat{\phi}_\ell = \frac{1}{\ell} \sum_{t=1}^{\ell} \xi_{i_t} \,, \tag{1}$$

where the ξ_i are quenched random variables associated with the vertices $i = 1, \ldots, N$ of the graph, which could be independent of, be correlated with, or be deterministic functions of the degrees k_i of the vertices. It is expected that the $\hat{\phi}_\ell$ are for large ℓ sharply peaked about their mean

$$\bar{\phi}_\ell = \frac{1}{\ell} \sum_{\mathbf{i}_\ell} P(\mathbf{i}_\ell) \sum_{t=1}^{\ell} \xi_{i_t} = \left\langle \frac{1}{\ell} \sum_{t=1}^{\ell} \xi_{i_t} \right\rangle \tag{2}$$

where $P(\mathbf{i}_\ell)$ denotes the probability of the path $\mathbf{i}_\ell$.

The average (2) can be obtained from the *cumulant generating function*

$$\psi_\ell(s) = \frac{1}{\ell} \ln \sum_{\mathbf{i}_\ell} P(\mathbf{i}_\ell) \, \mathrm{e}^{s \sum_{t=1}^{\ell} \xi_{i_t}} \tag{3}$$

as $\bar{\phi}_\ell = \psi'_\ell(s)|_{s=0}$. Here, we are interested in rare events, for which the empirical averages $\hat{\phi}_\ell$ take values ϕ which differ significantly from their mean $\bar{\phi}_\ell$. Large deviation theory predicts that for $\ell \gg 1$ the probability density $P(\phi)$ for such an event scales exponentially with path-length ℓ, i.e. $P(\phi) \sim e^{-\ell I(\phi)}$, with a *rate function* $I(\phi)$ which, according to the Gärtner-Ellis theorem [14], is obtained as a Legendre transform

$$I(\phi) = \sup_s \{s\phi - \psi(s)\} \tag{4}$$

of the limiting cumulant generating function $\psi(s) = \lim_{\ell\to\infty} \psi_\ell(s)$, provided that this limit exists and that it is differentiable. We shall see that the second condition may be violated, and that the derivative $\psi'(s)$ may develop discontinuities at certain s-values, entailing that we observe regions where the Legendre transform of $\psi(s)$ is strictly linear and only represents the convex hull of the true rate function [14].

2.2. Formulation in terms of deformed transition matrices

In order to evaluate $\psi_\ell(s)$, we express path probabilities using the Markov transition matrix W and a distribution $\mathbf{p}_0 = (p_0(i_0))$ of initial conditions as $P(\mathbf{i}_\ell) = [\,\prod_{t=1}^{\ell} W_{i_t i_{t-1}}]\, p(i_0)$, entailing that $\psi_\ell(s)$ can be evaluated in terms of a deformed transition matrix $W(s) = (e^{s\xi_i} W_{ij})$ as $\psi_\ell(s) = \ell^{-1} \ln \sum_{i_\ell, i_0} [W^\ell(s)]_{i_\ell i_0}\, p(i_0)$. Using a spectral decomposition of the deformed transition matrix one can write this as

$$\psi_\ell(s) = \ln \lambda_1 + \frac{1}{\ell} \ln \left[(\mathbf{1}, \mathbf{v}_1)(\mathbf{w}_1, \mathbf{p}_0) + \sum_{\alpha(\neq 1)} \left(\frac{\lambda_\alpha}{\lambda_1}\right)^{\ell} (\mathbf{1}, \mathbf{v}_\alpha)(\mathbf{w}_\alpha, \mathbf{p}_0) \right]. \tag{5}$$

Here the $\lambda_\alpha = \lambda_\alpha(s)$ are eigenvalues of $W(s)$, the $\mathbf{v}_\alpha$ and $\mathbf{w}_\alpha$ are the corresponding right and left eigenvectors, $\mathbf{1} = (1, \dots, 1)$, and the bracket notation $(\cdot, \cdot)$ is used to denote the standard inner product. Eigenvalues are taken to be sorted in decreasing order $\lambda_1 \geq |\lambda_2| \geq |\lambda_3| \ldots \geq \lambda_N$, with the first inequality being a consequence of the Perron-Frobenius theorem [15].

For long paths, the value of the cumulant generating function is dominated by the leading eigenvalue $\lambda_1 = \lambda_1(s)$ of $W(s)$, so $\psi(s) = \log \lambda_1(s)$. When computing $\lambda_1(s)$, it is advantageous for the purpose of computational efficiency and stability to exploit the fact that $W(s)$ can be symmetrised by a similarity transformation involving a diagonal matrix $D = \mathrm{diag}\,(\max\{k_i, 1\} \times e^{s\xi_i})$ constructed in terms of the s dependent 'deformation factors' $e^{s\xi_i}$ and the vertex degrees k_i,

$$\tilde{W}(s) = D^{-1/2} W(s) D^{1/2}\,. \tag{6}$$

The symmetrised matrix has elements

$$\tilde{W}_{ij}(s) = e^{\frac{s}{2}\xi_i}\, \frac{a_{ij}}{\sqrt{k_i k_j}}\, e^{\frac{s}{2}\xi_j} \tag{7}$$

and the same eigenvalues as $W(s)$. Note that, appart from the appearance of the deformation factors, this symmetrization (via a similarity transform) is the standard symmetrization procedure for reversible Markov matrices, based on the equilibrium distribution. The above equation simply expresses the fact that this symmetrization also works for $s \neq 0$, i.e. with deformation factors present.

Denoting by $\tilde{\mathbf{v}}_1 = \tilde{\mathbf{v}}_1(s)$ the (normalised) eigenvector corresponding to the algebraically largest eigenvalue λ_1 of $\tilde{W}(s)$, thus of $W(s)$, we have

$$\lambda_1 = (\tilde{\mathbf{v}}_1, \tilde{W}(s)\,\tilde{\mathbf{v}}_1)\,, \tag{8}$$

This identity allows one to use standard first order perturbation theory to express the derivtive $\psi'(s)$ required to find the supremum in Eq. (4) algebraically as

$$\psi'(s) = \frac{1}{\lambda_1}(\tilde{\mathbf{v}}_1, \tilde{W}'(s)\,\tilde{\mathbf{v}}_1) = \frac{1}{\lambda_1}\sum_{i,j}\tilde{v}_{i,1}\frac{\xi_i + \xi_j}{2}\tilde{W}_{ij}(s)\tilde{v}_{j,1} = \sum_i \xi_i \tilde{v}_{i,1}^2\,. \tag{9}$$

In the first equality above we have exploited the fact that $(\tilde{\mathbf{v}}_1'(s), \tilde{\mathbf{v}}_1(s)) = (\tilde{\mathbf{v}}_1(s), \tilde{\mathbf{v}}_1'(s)) = 0$, which is a consequence of the s-independent normalization of eigenvectors; in the second equality the expression of $\tilde{W}'(s)$ is inserted, and the last equation exploits the eigenvector property of $\tilde{\mathbf{v}}_1$, and the symmetry of the previous expression under $i \leftrightarrow j$ interchange to obtain the final expression.

This concludes the general framework. For the remainder of this paper, we will restrict our attention to the case where $\xi_i = f(k_i)$, with f an arbitrary function of the degree.

Note that in the $s = 0$ case, the eigenvalue problem is trivial, as the column-stochasticity of the transition matrix yields a left eigenvector $w_i \equiv 1$ corresponding to the maximal eigenvalue $\lambda_1 = 1$. The associated right eigenvector is $v_i \propto k_i$. For nonzero s, such closed form expressions are in general not known. Performing a direct matrix diagonalisation can be quite daunting for large system sizes N, even if one exploits methods that are optimised to calculate only the first eigenvalue [16]. Hence we are interested in fast viable approximations. In the next subsection we describe one such approximation expected to be valid for networks in which vertex degrees are typically large.

2.3. Degree-based approximation.

We start by considering the left eigenvectors $\mathbf{w}$ instead of the right eigenvectors, for which the eigenvalue equation can be written as

$$\lambda\, w_j = \frac{1}{k_j}\sum_{i\in\partial j} w_i\, \mathrm{e}^{sf(k_i)}\,. \tag{10}$$

This system of equations can be simplified by considering a degree-based approximation for the first eigenvector, where one assumes that the values of w_i only depend on the degree of the node i: $w_i = w(k_i)$. If the smallest degree k_j appearing in Eq (10) is large enough, we can write the eigenvalue equation (10) by appeal to the law of large numbers as

$$\lambda_1(s)\, w(k) = \sum_{k'} P(k'|k)\, w(k')\, e^{sf(k')} \tag{11}$$

where $P(k'|k)$ is the probability for the neighbour of a node of degree k to have degree k'. For ER graphs this approximation is expected to work well at sufficiently large mean degree. In graphs with power law behaviour of their degree distributions at large k, one would have to put a large lower cutoff on the degrees appearing in the system.

In an Erdős-Rényi ensemble [17], and more generally in any configuration model ensemble, we have $P(k'|k) = P(k')\frac{k'}{\langle k \rangle}$. In this case the right-hand side of (11) does not depend on k and the $w(k)$ are in fact k-independent. The eigenvalue equation then simplifies to

$$\lambda_1(s) = \left\langle \frac{k}{\langle k \rangle} e^{sf(k)} \right\rangle , \qquad (12)$$

where the average is over the degree distribution $P(k)$. This approximation yields excellent results for large mean connectivities $c = \langle k \rangle$ on ER graphs, and more generally for configuration models without low degree nodes. This is illustrated in figure 1, where we plot a comparison with numerical simulations for ER graphs with $c = 30.$ and for SF graphs with $c = 40$. While the occurrence of low degree vertices is not strictly excluded in either system, we find that the probability of having vertices with $k_i < 20$ is sufficiently small in both systems to render the degree based approximation very reasonable in both cases. In figure 1 and throughout the remainder of the paper simulation results are obtained as averages over 1000 samples, unless explicitly stated otherwise.

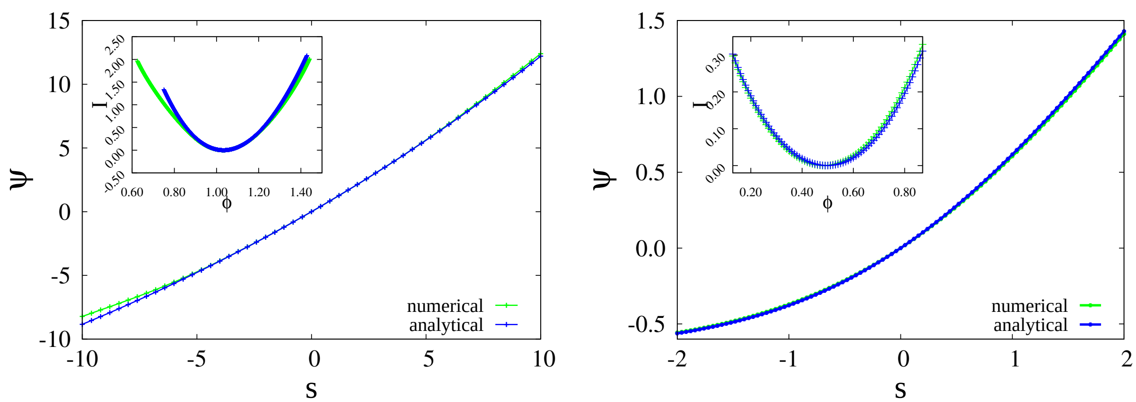

Figure 1. (Colour online) Cumulant generating function $\psi(s)$, comparing the large-degree approximation (12) (blue line) with results of a numerical simulation (green line). Left panel: result for ER networks with $c = 30$ and $f(k_i) = k_i/c$. Right panel: result for scale free graphs with $c = 40$ and $f(k_i) = \Theta(c - k_i)$. In both cases the inset shows the corresponding rate functions.

2.4. *Eigenvector localisation.*

Because of the heterogeneity of the underlying system, one finds that the random walk transition matrix typically exhibits localised states, both for fast and slow relaxation modes [18], even in the undeformed system, although the eigenvector corresponding to the largest eigenvalue (the equilibrium distribution) will typically be delocalised. However, given the nature of the deformed transition matrix, one expects the deformed random walk for large $|s|$ to be localised around vertices where $sf(k_i)$ is very large; hence we anticipate that in the deformed system, even the eigenvector corresponding to the largest eigenvalue *may* become localised for sufficiently large $|s|$. In order to investigate this effect quantitatively we look at the inverse participation ratio of the eigenvector corresponding to the largest eigenvalue λ_1 of $W(s)$. Denoting by v_i its i-th component, we have

$$\mathrm{IPR}[\mathbf{v}] = \frac{\sum_i v_i^4}{\left[\sum_i v_i^2\right]^2} \tag{13}$$

One expects $\mathrm{IPR}[\mathbf{v}] \sim N^{-1}$ for a delocalised vector, whereas $\mathrm{IPR}[\mathbf{v}] = O(1)$ if $\mathbf{v}$ is localised.

The situation is somewhat subtle in scale free systems. Although the equilibrium distribution given by the eigenvector corresponding to the eigenvalue $\lambda_1 = 1$ in the undeformed system at $s = 0$, i.e. $v_i \propto k_i$, has support in the *entire* system, the IPR of that eigenvector does not exhibit a $1/N$ scaling expected for a (fully) delocalised state. This is due to the fact that both sums appearing in the definition (13) of the IPR will fail to converge in the infinite system limit, if the degree distribution has a sufficiently slow power law decay, as indeed in the SF system considered here for which $P(k) \sim k^{-3}$ for large k. In that case the IPR will still decay to zero in the large system limit, but at a rate $\mathrm{IPR}[\mathbf{v}] \sim 1/[N^{1/3}(\log N)^2]$, i.e. much slower than $1/N$, entailing that the equilibrium state "effectively" lives on a sub-extensive fraction of the system.

3. Results on random graphs

We performed numerical simulations to evaluate $\lambda_1(s)$ and the $\mathrm{IPR}[\mathbf{v}_1(\mathrm{s})]$ for several types of network, defined by their random graph topology. In the present paper we restrict ourselves to discussing results for Erdős-Rényi (ER) and for scale free (SF) networks. We found that other network ensembles give qualitatively similar results.

As to the function $f(k_i)$, we also looked at various examples. In what follows we will report results for the normalised degree $f(k_i) = k_i/c$, and for the binary function $f(k_i) = \Theta(c - k_i)$. Although details do of course depend on the precise nature of the function chosen we find that — qualitatively — other deterministic types of degree-dependent function exhibit analogous behavior. In the case of ER networks, we restrict our simulations to the largest (giant) component of the graphs, in order to prevent spurious effects of isolated nodes or small disconnected clusters (e.g. dimers) dominating $\lambda_1(s)$ and the IPR for large $|s|$, as these would represent trivial instances of rare events, where a walker starts, and is thus stuck on a small disconnected component of the graph. From here on, the network size of ER graphs given must be understood as the size of the networks from which the giant component is extracted. The SF networks we have been looking at so far are created by a process of preferential attachment; they are thus simply connected by construction.

Fig. 2 reports results for ER graphs of mean degree $c = 6$ and $f(k_i) = k_i/c$. From the behaviour of the IPRs. we can read off the existence of two localised regimes for sufficiently large values of $|s|$, with IPRs on the localised side of both transitions increasing with system size. Results can be understood, as for large $|s|$ the deformed random walk is naturally attracted to the nodes with the largest (resp. smallest) degrees for positive (resp. negative) s. Thus for large negative s the deformed walk tends to be concentrated at the end of the longest dangling chain, whereas for large positive s it will be concentrated at the site with the largest available degree. On an ER network where the large-degree tail of the degree distribution decays very fast, such a high degree vertex is likely to be connected to vertices whose degrees are lower, even significantly lower, than that of the highest degree vertex in the network, which leads to IPRs approaching 1 in the large N limit. Conversely, for negative s, the deformed random walk will be attracted to the ends of dangling chains in the network, with the probability of escape from a chain decreasing with its length (with the length of the longest dangling chain increasing with system size). This can explain that IPRs initially saturate at 1/2 for large systems. Only upon further decreasing s to more negative values will the asymmetry of the deformed transition probabilities, to and away from the end of a dangling chain, induce that further weight of the dominant eigenvector becomes concentrated on the end-site, leading to a further increase of the IPR.

From the values of $\lambda_1(s)$ we also derived the large deviation rate functions $I(\phi)$ for this system. They are reported in the right panel of Fig. 2. While the right branch of $I(\phi)$ is for large N well approximated by a parabola, our results show the emergence of a linear region on the left branch, which becomes more pronounced as the system size is increased. This is a signature of a non-differentiable point of $\psi(s)$ at a point s^* estimated to be at $s^* \simeq -0.307$: at this point the Gärtner-Ellis theorem cannot be used to evaluate the rate function, and the linear branch only represents the convex envelope of the true $I(\phi)$ [14]. The latter can either coincide with its convex envelope, or it can indeed be non-convex. However this information cannot be accessed by the theorem. The emergence of a jump-discontinuity in $\psi'(s)$ is due to a level crossing of the two largest eigenvalues, where the system switches between two modes that correspond to the largest eigenvalue on either side of s^*. In finite systems the crossing is an "avoided crossing" due to level repulsion, but the two largest eigenvalues

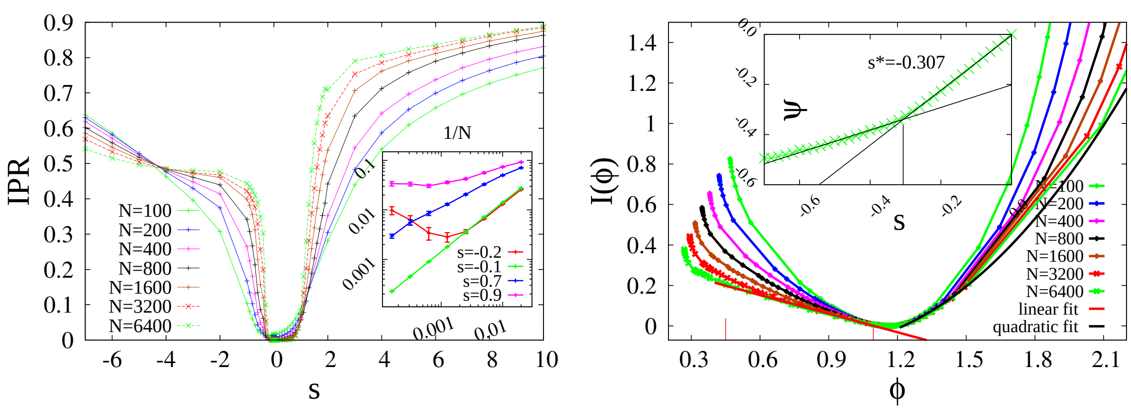

Figure 2. Left panel: IPRs as functions of the deformation parameter s for ER graphs with $c = 6$, and $f(k_i) = k_i/c$, for system sizes ranging from $N = 100$ to $N = 6400$. The inset exhibits the N^{-1}-scaling of IPRs for 4 different values of the deformation parameter s, chosen in pairs on either side of *two* localisation transitions, one at negative, and one at positive s. Right panel: Large deviation rate function $I(\phi)$ for this system. For the largest system size, a linear fit of the convex envelope of the left branch and a quadratic fit of the right branch of $I(\phi)$ are shown as well. In the inset of the right panel, we show $\psi(s)$ in the vicinity of the non-differentiable point.

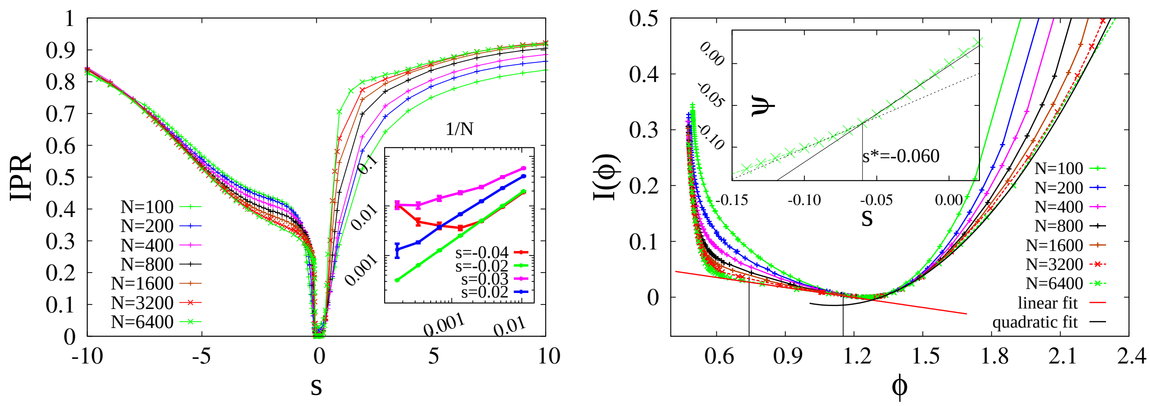

Figure 3. IPRs (left panel) and rate function $I(\phi)$ (right panel) for ER graphs with $c = 3$, and $f(k_i) = k_i/c$ for system sizes ranging from $N = 100$ to $N = 6400$. As in Fig 2 we include an inset in the left panel which shows the scaling of IPRs with system size N for 2 pairs of values of the deformation parameter s, each pair being chosen so as to approximately bracket the location of a localisation transition. The plot of the rate function in the right panel also shows linear fit of the convex envelope of the left branch and a quadratic fit of the right branch of $I(\phi)$ for the largest system size, as well as a plot of $\psi(s)$ in the vicinity of the non-differentiable point in an inset.

become asymptotically degenerate at s^* in the $N \to \infty$ limit.

In Fig 3 we report analogous results for the same problem, but now on an ER network at the lower connectivity of $c = 3$, where we see the same set of phenomena: delocalised states at low $|s|$ becoming localised as $|s|$ is increased, as witnessed by the behaviour of the IPRs. Due to the larger heterogeneity of the low-c system, the region of extended states is confined to a narrower region on the s axis than in the case of the $c = 6$ system. As in the $c = 6$ system, we also observe a jump discontinuity of $\psi'(s)$ emerging at large system size, which gives rise to a linear branch in the plots of the rate function. In the present case we locate the discontinuity at $s^* \simeq -0.060$.

Let us now turn to looking at rare events for random walks on scale free graphs. Here we present results for SF networks with mean degree $c = 4$ which are generated using a preferential attachment algorithm. It creates graphs with a degree distribution which behaves as $P(k) \sim k^{-3}$ at large k. Any realisation is thus likely to contain vertices with very large degrees. In order to avoid numerical complications arising from huge dynamical ranges of deformed transition matrix elements $W_{ij}(s) = \mathrm{e}^{sf(k_i)} W_{ij}$, we restrict ourselves to looking at a function f which remains bounded at large k_i. Our choice here is $f(k_i) = \Theta(c - k_i)$. We are thus looking at rare events characterised by random walkers visiting atypically many vertices with degree below the average degree c.

In Fig 4 we report results for this system in the same manner as above for the ER graphs. The IPRs clearly indicate localisation at large positive s, as we find IPRs increasing with system size. Conversely, at large negative s, we find IPRs slowly decreasing with system size. Whether asymptotic IPRs would remain $O(1)$ in the infinite system limit or decrease very slowly with N in a manner expected for the $s = 0$ case is difficult to discern from the system sizes currently available to us. Thus we will have at least one, possibly also two localisation transitions in the present system, provided that we are prepared to classify the $s = 0$-state as delocalised. We recall our earlier discussion of the subtleties of this case in Sec 2.4. As to the rate function $I(\phi)$, we also find it to develop a linear branch associated with an emerging non-analyticity of the cumulant generating function $\psi(s)$ which we now locate at a positive s value, viz. at $s^* \simeq 0.543$. As in the ER case, this feature can be traced to a mode-switching transition in the system.

Concerning the infinite sytem limit of the results presented above, it is indeed expected that the largest eigenvalue $\lambda_1(s)$, and thereby (the convex envelope of) the rate function will in all cases presented converge in this limit (in the sense that the distribution of $\lambda_1(s)$ becoming sharp as $N \to \infty$). As is evident from our results, there are, however, still notable finite size corrections at the system sizes available to our simulations. Here, recent results allowing to obtain the maximum eigenvalue of sparse symmetric matrices analytically [19] could be used to make further progress.

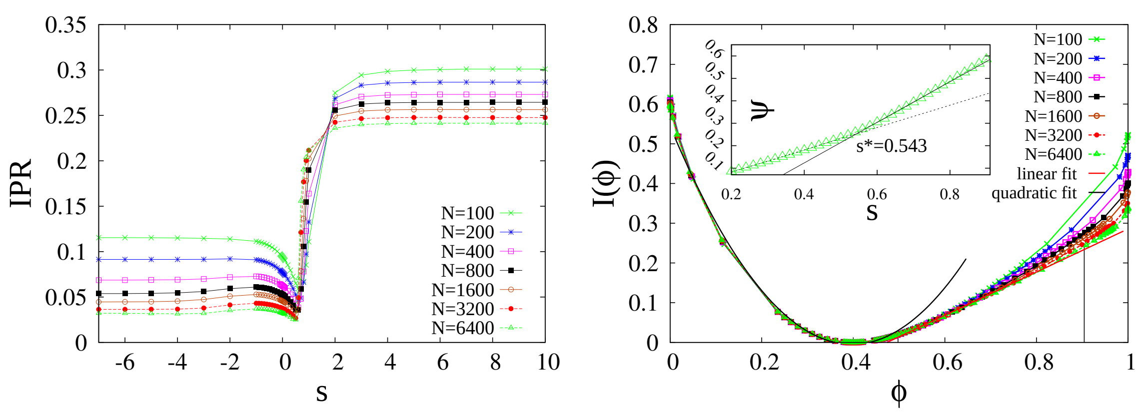

Figure 4. IPRs (left panel) and rate function $I(\phi)$ (right panel) for scale free graphs with $c = 4$, and $f(k_i) = \Theta(c - k_i)$ for system sizes ranging from $N = 100$ to $N = 6400$. For the largest system size, a linear fit of the convex envelope, now of the *right* branch and a quadratic fit of the left branch of $I(\phi)$ are also shown. In the inset of the right panel, we show $\psi(s)$ in the vicinity of the non-differentiable point.

Let us finally turn to a more detailed discussion of the mode-switching transitions characterised by the emergence of a non-analyticity of the cumulant generating function $\psi(s)$ in the large system limit, more specifically an emergent jump discontinuity of $\psi'(s)$, which we have observed both in ER networks for $f(k_i) = k_i/c$ and in SF networks for $f(k_i) = \Theta(c - k_i)$. These transitions are related to level crossings, which are avoided in finite systems due to level repulsion. As the system size increases the two largest eigenvalues of the system will become asymptotically degenerate at the point of the avoided level crossing. As a consequence, we expect this mode-switching transition to give rise to a divergence of the correlation length

$$\xi(s) = [\ln(\lambda_1(s)/\lambda_2(s)]^{-1} \tag{14}$$

at s^* in the infinite system limit, in close analogy with phenomenology of second order phase transitions. In finite systems, the divergence will be rounded, but a peak is expected to evolve near s^*, with the peak height and the distance of the peak from s^* scaling with system size. We find that the divergence of the peak height is logarithmic in N in the present case. This form of the divergence is *also* completely analogous to that observed for critical correlation lengths in standard second order phase transitions, i.e. it is proportional to the linear scale of the system: indeed, for graphs the analogy of the linear scale of the system would be the graph-diameter, which is well known to scale logarithmically in system size N.

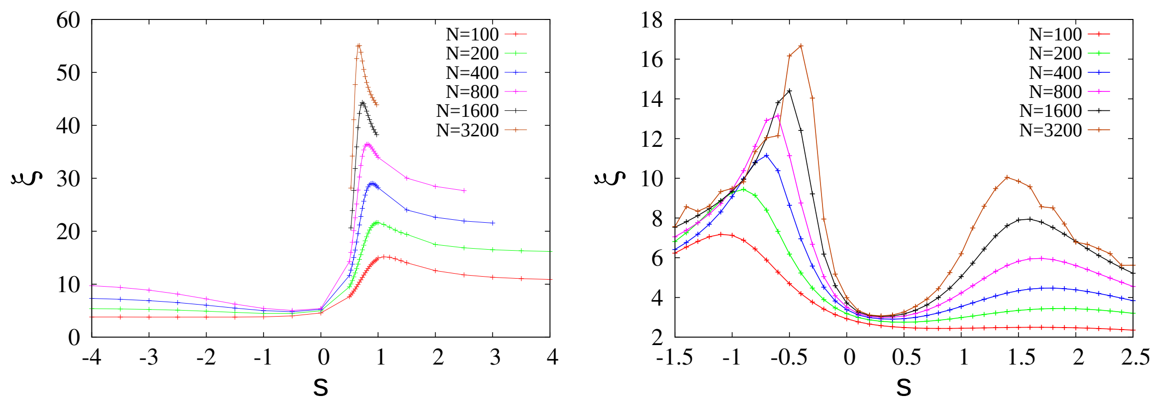

Figure 5. Correlation length $\xi(s)$ for scale free graphs with $c = 4$ and $f(k_i) = \Theta(c - k_i)$ (left panel), and for ER graphs with $c = 6$ and $f(k_i) = k_i/c$ (right panel). In both panels, system sizes range from $N = 100$ to $N = 3200$ (bottom to top curves). For SF graphs one sees a peak emerging with peak positions converging to a value s^* compatible with that found from the emerging non-analyticity of $\psi(s)$ in Fig 4, and peak heights scaling like $\log N$. For the ER graphs we observe a *second* peak with peak position converging to $s^* = 1.1 \pm 0.3$ in addition to the one expected from the non-analyticity of $\psi(s)$ observed in Fig 2. Heights of both peaks increase logarithmically in N.

In Figure 5 we report results for the s dependent correlation lengths for the two types of systems looked at above, SF networks with $f(k_i) = \Theta(c - k_i)$ and ER networks with $f(k_i) = k_i/c$. While position of the emerging peak in $\xi(s)$ for the former case is compatible with the location of the asymptotic jump-discontinuity observed in $\psi'(s)$ we find a second peak emerging in the case of the ER network with peak height *also* diverging logarithmically in N. The corresponding emerging second point of divergence of $\xi(s)$ has been difficult to discern from the behaviour of $\psi(s)$ for the the available system sizes: although we expect a second emerging jump discontinuity of $\psi'(s)$ and thus a second linear branch of the Legendre transform of $\psi(s)$) to be associated with it, it appears that the size of that jump (and thus the extent of the second linear region of $I(\phi)$) are too small to be discernible at the system sizes available to our simulations.

Preliminary results indicate that the emergence of *two* non-analyticities rather than one is related to the function f rather than to the network topology: we have seen a single peak (rather than two) emerging for ER graphs with $f(k_i) = \Theta(c - k_i)$ as the observable for which large deviations of path-averages are investigated.

4. Conclusions and future perspectives

In this paper we have analysed rare events statistics for path averages of observables associated with sites visited along random walk trajectories on complex networks. Results are obtained by looking at spectral properties of suitably deformed transition matrices. The main outcome of our analysis is the possible emergence of two types of dynamical phase transitions in low mean degree systems: localisation transitions which entail that large deviations from typical values of path averages may be realised by localised modes of a deformed transition matrix, and *mode-switching transitions* signifying that the modes (eigenvectors) in terms of which large deviations are typically realised may switch as the deformation parameter s and thus the actual scale of large deviations are varied. Results of numerical simulations consistently support these claims. We also developed an analytical approximation valid for networks in which degrees are typically large.

While we have restricted ourselves in the present investigation to analysing unbiased random walks, it is clear that the method of deformed transition matrices is not restricted to this case [14, 13] and is easily extended to more general stochastic processes, including indeed irreversible ones. For irreversible processes the symmetrization of transition matrices is not available, and one would have to work directly with the non-symmetric versions. In that case algebraic expressions for the derivative of the cumulant generating function of the type Eq. (9) are still available, but they would involve the use of left and right eigenvectors of the original matrix, rather than eigenvectors of a symmetrized version.

Our work opens up the perspective to study a broad range of further interesting problems. On a technical level, one would want to implement more powerful techniques, such as derived in [19], to obtain the largest eigenvalue in the present problem class for larger system sizes, and indeed in the thermodynamic limit $N \to \infty$. Then there is clearly the need to systematically study the dependence of the phenomena reported here on the degree statistics, and on the nature of the observables for which path averages are looked at. We have gone some way in this direction, but intend to report further results in the future. In particular one might wish to look at observables which, rather then being deterministic functions of the degree, are only statistically correlated with the degree, or at observables taking values on *edges between nodes* [14, 13]. This could be of interest in applications such as traffic or information flows on networks subject to capacity constraints on edges. Moreover, given the nature of the mode-switching transition observed in the present paper, it is clearly conceivable that *several such transitions* could be observed in a single system, depending of course on the nature of the observables studied and on the topological properties of the underlying networks. Indeed for path averages of the degrees of vertices visited, our results indicate the existence of two such transitions, whereas for $f(k_i) = \Theta(c-k_i)$ we have seen only a single transition. Finally, critical phenomena associated with the localisation transition and with mode-switching transitions also deserve further study. We believe that this list could go on.

Let us, however, emphasise that our investigation of rare events statistics for random walks on networks constitutes only the the beginning of a story. For practical applications in particular, rare events statistics of observables other than the simple path averages of the type considered in the present paper would be needed: in the context of cyber-security and hide-and-seek games, for insance, one would be interested in the statistics of the number of *different* (tagged) sites visited by a random walker. While typical results for this number could be obtained by a relatively straightforward modification of the approach proposed in [20], obtaining the corresponding large deviation properties may turn out to be more involved. Note, however, that localisation transitions could be relevant in that problem, too, if indeed finding unusually large numbers of different tagged sites requires that a random walker becomes localised on the subset of tagged sites.

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