

## Maximal dispersion of adaptive random walks

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Maximum entropy random walks (MERWs) are maximally dispersing and play a key role in optimizing information spreading in various contexts. However, building MERWs comes at the cost of knowing beforehand the global structure of the network, a requirement that makes them totally inadequate in real-case scenarios. Here, we propose an adaptive random walk (ARW), which instead maximizes dispersion by updating its transition rule on the local information collected while exploring the network. We show how to derive ARW via a large-deviation representation of MERW and study its dynamics on synthetic and real-world networks.

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In the last decade we have assisted with a wave of new works studying extreme (rare) events associated to dynamical processes evolving on complex networks [1–17]. The necessity to understand unlikely events comes from the fact that, although rare, their appearance determines the future of the system under study, which may be potentially catastrophic, e.g., earthquakes [1]. In this context, researchers have focused on random walks and their load and flow properties [2,3,15,17] for models of traffic in transportation [11,16] and communication networks [4], or on epidemic models and extinction events [6], or again on general order-disorder [8] and percolation transitions [9,10] to corroborate the robustness of networks. In these settings, rare events are often driven by internal noise, and their understanding could provide us with control mechanisms to keep away from harmful scenarios [5,6,8,10].

Among all dynamical processes evolving on networks, discrete-time biased and unbiased random walks (URWs) stand out as simple and insightful models of diffusion processes on discrete topologies [18].

A fundamental property of random walks is their ability to *homogeneously* spread over the whole network. Mathematically, the spreading capability of a random walk can be characterized by measuring the entropy production rate. In many scenarios, it is indeed of uttermost importance to design random walks that maximise such entropy production rate in order to spread the most homogeneously. To picture this, imagine having equal-size groups of random walks

with different colors running on a network; at each time, the most homogeneous spreading is obtained with an equal proportion of colors on every node. Such a well mixing, or maximal dispersion, turns out to be particularly useful when information about a node state (e.g., its healthy or infected condition, its availability, etc.) needs to be homogeneously spread to all other nodes in the network [19–21], a sought after property for transportation and ad-hoc networks [22]. It is known that a random walk achieves maximal dispersion when it travels all trajectories of the same length with uniform probability. Such a property characterises the so-called maximum entropy random walk (MERW) [20,23] and is used in a myriad of practical cases: testing network robustness [24,25] and navigability [26–29], predicting links and communities [30–33] as well as disease associations [34], or assessing neutral quasispecies evolution in biology [35], to name a few. However, in order to build MERW, it is required to know the topology of the whole network before even exploring it [20,21,23]. Apart from the expensive computational cost of defining the stepping rule of MERW (based on calculating dominant eigenvalue and eigenvector of a  $N \times N$  matrix, with  $N$  the number of nodes), having global knowledge of the network beforehand is an heavy drawback that makes MERW totally inadequate on networks whose structure cannot be entirely determined *a priori* or changes over time (e.g., growing networks [36] or temporal networks [37,38]). It is therefore fundamental to optimally design dispersive random walks that just make use of local information while exploring the network. Several attempts have been made in this direction, although so far finding only *approximate* solutions (see, for example, Ref. [21]).

In this Letter, we solve this longstanding problem by proposing an adaptive random walk (ARW) that *locally* updates its stepping rule based on the structure of the explored network. Without requiring any prior knowledge of the whole topology, ARW outperforms MERW, as it is maximally

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dispersive on every portion of the network visited and not only on the whole graph. Via a bridge between large-deviation theory and network science, MERW can be seen as a rare event of URW. We exploit this to construct ARW as a single-trajectory rare event sampling algorithm [39,40] that only makes use of local information available to adapt itself—changing its transition probabilities step by step—in order to best spread on the network. Shaping the random walk by only gathering local information is an outstanding property that makes ARW the only sensible choice for optimising the spreading on networks with time-varying topology and on heterogeneous networks. Indeed, imagine having a network composed by two main modules, connected to each other and topologically very different. MERW initialised on one of the modules is not able to maximise dispersion while exploring it as its stepping rules are based on the “averaged” structure of the whole network. On the contrary, ARW is optimally dispersive in every exploration phase. In the following, this is made evident by showing that ARW has an entropy production rate closer to the maximal one on the visited portion of the graph if compared with URW and MERW. Moreover, when the network is fully explored, ARW and MERW have similar mixing properties and, in the thermodynamic limit, they become the same.

We start by considering an URW  $X = (X_1, X_2, \dots, X_n)$  on a finite connected and undirected graph  $G = (V, E)$  characterized by a set of nodes  $V$  and a set of links  $E$ . The topology of the graph is encoded in the adjacency matrix  $A = \{a_{ij}\}$ , where  $a_{ij} = 1$  if the nodes  $i$  and  $j$  are connected, and  $a_{ij} = 0$  otherwise. We also define the degree of node  $i$  as  $k_i = \sum_{j \in V} a_{ij}$ . URW dynamics is determined by the stochastic transition matrix  $\Pi_U$ , with components

$$(\pi_U)_{ij} = \frac{a_{ij}}{k_i}, \quad (1)$$

describing the probability of URW to move from  $X_\ell = i$  at time  $\ell$  to  $X_{\ell+1} = j$  at time  $\ell + 1$ . We focus on a particular dynamic observable that characterises the entropic content of a random walk trajectory,

$$C_n = \frac{1}{n} \sum_{\ell=1}^n \ln k_{X_\ell}. \quad (2)$$

Indeed, apart from boundary terms that do not influence our discussion,  $C_n$  is the logarithm of the probability of URW trajectory divided by the number of time steps  $n$ . Noticeably, by taking the long-time limit of the average over all paths of  $C_n$ , we get the so-called Kolmogorov-Sinai entropy production rate  $h_U$  [20,21,41], i.e.,  $h_U = \lim_{n \rightarrow \infty} \langle C_n \rangle$ , interpreted as the mean information generated per time step. For a generic ergodic random walk, it can be written as

$$h = - \sum_{i,j} \rho_i \pi_{ij} \ln \pi_{ij}, \quad (3)$$

where  $\rho = \{\rho_i\}$  and  $\pi = \{\pi_{ij}\}$  are the stationary distribution and the transition probability matrix of the random walk. Eventually, the observable  $C_n$  is a random variable of the random walk process that represents the fluctuating version of  $h_U$ , viz., the fluctuating trajectory entropy [42,43].

The finite-time fluctuating nature of  $C_n$  around its typical value  $h_U = \sum_{i \in V} \rho_i \ln k_i$  is of interest here. A complete

understanding of the fluctuations is given by the probability density  $P_n(c) := P(C_n = c)$ , which is known to have the large-deviation form

$$P_n(c) = e^{-nI(c)+o(n)}, \quad (4)$$

with the non-negative large-deviation rate function  $I(c)$  characterizing the leading behavior of  $P_n(c)$  and  $o(n)$  denoting corrections smaller than linear in  $n$ . The focus thus moves onto studying  $I$  in Eq. (4), which has a unique zero at  $c^* = h_U$ . The rate function can be calculated by means of the so-called Gärtner-Ellis theorem [43–45], which states that  $I$  is given by the Legendre-Fenchel transform of the scaled cumulant generating function (SCGF)

$$\Psi(s) = \lim_{n \rightarrow \infty} \frac{1}{n} \ln \mathbb{E}[e^{nsC_n}], \quad (5)$$

as this last is differentiable for a finite graph [45]. In particular, as URW is an ergodic Markov process, the SCGF can be obtained as

$$\Psi(s) = \ln \zeta_s, \quad (6)$$

where  $\zeta_s$  is the dominant eigenvalue of the so-called tilted matrix  $\tilde{\Pi}_s = \{(\tilde{\pi}_s)_{ij}\}$ , with components

$$(\tilde{\pi}_s)_{ij} = \pi_{ij} e^{s \ln k_i} = \pi_{ij} k_i^s = a_{ij} k_i^{s-1}. \quad (7)$$

Hence, the likelihood of fluctuations can be studied using the SCGF  $\Psi$  rather than the rate function  $I$ .

However, calculating the probability of fluctuations is only a first step towards the prediction and control of rare events. It is indeed important to also understand how these extreme events are created in time. In this context, we construct the driven process [46–48] associated with a given fluctuation  $C_n = c$ . This process is a locally biased version of URW [12,47] and its transition probability matrix is given by

$$(\pi_s)_{ij} = \frac{(\tilde{\pi}_s)_{ij} r_s(j)}{r_s(i) \zeta_s} = \frac{a_{ij} k_i^{s-1} r_s(j)}{r_s(i) \zeta_s}, \quad (8)$$

where  $r_s$  is the right eigenvector associated with  $\zeta_s$ . The driven process is still Markovian and ergodic and can be interpreted as the effective dynamics of the subset of paths of URW leading to a fluctuation  $C_n = c$  [12,13,47]; to match such a fluctuation [49], the Laplace parameter  $s$  must satisfy

$$c = \Psi'(s). \quad (9)$$

Eventually, the entropy rate of the driven process can be obtained taking Eq. (8) and plugging it into Eq. (3) and can be expressed in terms of the SCGF [12] as

$$h(s) = \Psi(s) + (1-s)\Psi'(s). \quad (10)$$

In Sec. II of the Supplemental Material (SM) [63] we show that  $h(s)$  in Eq. (10) has a global maximum for  $s = 1$ , i.e.,

$$h(1) = \Psi(1) = \ln \zeta_1, \quad (11)$$

where  $\zeta_1$  is the dominant eigenvalue of the adjacency matrix  $A$ . Replacing  $s = 1$  in the driven process, Eq. (8) gives MERW

$$(\pi_1)_{ij} = \frac{a_{ij} r_1(j)}{r_1(i) \zeta_1}, \quad (12)$$

allowing us to interpret MERW on a network as a biased random walk creating a rare event fluctuation—given by replacing  $s = 1$  in Eq. (9)—of URW [12].

This result shows, on the one hand, that we can sample a particular rare event of URW by simulating MERW and, on the other hand, that MERW can in principle be obtained from URW by opportunely conditioning on a certain rare event of the observable  $C_n$  in Eq. (2). The latter observation is key to introduce our adaptive random walk (ARW). As we will show in the following, such ARW, through successive local adaptations of URW, reaches maximum entropy while exploring the network, i.e., much before the entire graph has been visited, and eventually converges to MERW on the whole network. To construct ARW, we develop here an algorithm based on a rare event sampling scheme [39,40,50–53]. According to this, the random walk updates its transition probability matrix at each time step, in order to typically visit a specific rare event of URW, obtained fixing  $s = 1$  in Eq. (9). We refer the reader to Sec. I of the SM [63] for a general formulation of the sampling algorithm valid for all additive observables and  $s \in \mathbb{R}$ .

Formally, ARW is a discrete-time process  $Y = (Y_1, Y_2, \dots, Y_n)$ , where  $Y_n \in V$  is the position of ARW on the graph at time  $n$ . The core of ARW is based on an adaptive power method to solve the following dominant eigenvalue equation:

$$\tilde{\Pi}_1 r_1 = \zeta_1 r_1, \quad (13)$$

which is known to be cardinal to construct MERW in Eq. (12). More in detail, our adaptive power method simulates single Markov chain transitions with importance sampling [54]. In particular, supposing that ARW is located on the node  $i$  at time  $n$ , i.e.,  $Y_n = i$ , the next step is proposed according to an estimate of MERW in Eq. (12) that reads

$$(\pi_1^{(n)})_{ij} = \frac{1}{Z} \frac{a_{ij} r_1^{(n)}(j)}{r_1^{(n)}(i) r_1^{(n)}(i_0)} = \frac{a_{ij} r_1^{(n)}(j)}{\sum_{j' \in V} a_{ij'} r_1^{(n)}(j')}, \quad (14)$$

where  $Z$  is the normalisation factor,  $i_0$  is an *a priori* fixed node, and  $r_1^{(n)}$  is the  $n$ th time estimate of the eigenvector centrality [39,40]. This last is given by the stochastic-approximation [55] formula

$$r_1^{(n+1)}(i) = r_1^{(n)}(i) + \lambda(n) \mathbf{1}_{Y_n=i} \left( \frac{\sum_{j \in V} a_{ij} r_1^{(n)}(j)}{r_1^{(n)}(i_0)} - r_1^{(n)}(i) \right), \quad (15)$$

based on an asynchronous update via the indicator function  $\mathbf{1}_{Y_n=i}$  and on the learning rate  $\lambda(n)$ . The indicator function selects the  $i$ th component of the eigenvector centrality to be updated only when the process  $Y$ , at the  $n$ th time step, has visited node  $i$ . Additionally, the learning rate  $\lambda(n)$ —commonly used in stochastic approximation protocols [50,51,55,56]—expresses how much of the information that has been learnt up to time  $n$  is used to update  $r_1$  in the next time step. Note that, in the following, all ARW simulations are obtained by using a learning rate  $\lambda(n) = 1/((n+1)^\beta)$ , with  $\beta = 0.1$ , in Eq. (15). Although there is no theory to *a priori* determine the learning rate, there are mathematical conditions that  $\lambda$  needs to satisfy, and one can carry out numerical simulations on benchmark networks to finely tune the value of  $\beta$ . We show how to do so in Sections III and VI of the SM [63] (see Fig. S2–S6,

Fig. S9, and Table S1), further noticing that our approach, in order to set off an ‘optimal’ value of  $\beta$ , does not require comparing the performance of ARW with MERW, or with any other spreading process that requires global knowledge of the network.

ARW is randomly initialized on a node of the network with a normalized random right eigenvector  $r_1^{(0)}$  and evolves according to the fully local rules in Eq. (14) and Eq. (15). At each time step it tends to optimize the spreading—aiming at maximum entropy production—on the portion of the network visited. In the long-time limit, it will eventually converge to MERW of Eq. (12) as  $r_1^{(n)} \rightarrow r_1$ ,  $r_1^{(n)}(i_0) \rightarrow \zeta_1$ , and  $Z \rightarrow 1$ . We insist on the fact that differently from MERW, ARW does not need to know the full topology of the network since the beginning, as it learns it on the run. Thanks to this, its entropy production rate stays always close to the maximum rate on the visited portion of the graph. This is drastically different from MERW which does not maximize the entropy while it explores the graph, but reaches optimal spreading only when the whole network has been visited.

We show this in Fig. 1(a)–1(c) where we compare the spreading properties of single trajectories of ARW, MERW, and URW on two network models, namely Erdős-Rényi, and Barabasi-Albert, and on a real-world manmade network. The last network describes an air transportation system: each node is a city and two nodes are connected if at least one air-plane flew between the two cities in the time window [11 Jan 2000–10 Jan 2001] [57]. In this last context, maximizing entropy production rate allows manufacturers, for example, to homogeneously spread goods around their factories. Each of the three processes is initialized on a randomly selected node of the network, and evolves according to its transition probability matrix. As the walker moves hopping through previously unvisited links, we calculate its entropy production rate  $h$  (solid line) and compare it with the optimal  $\bar{h}$  (dashed line) given by the logarithm of the dominant eigenvalue of the adjacency matrix associated with the portion of graph made by all (and only) previously visited links. The entropy production rate  $h$  of each process is calculated via a modified version of Eq. (3), that is

$$h(M) = - \sum_{(i,j) \in E(n)} \rho_i(M) \pi_{ij}(M) \ln \pi_{ij}(M). \quad (16)$$

This takes into account the number of visited links  $M = |E(n)|$  up to time  $n$ , where  $E(n)$  is the set of visited links,  $\pi_{ij}(M) = \pi_{ij} / (\sum_{(i,j') \in E(n)} \pi_{ij'})$  if the link  $(i, j)$  is in  $E(n)$ , while 0 otherwise, and the stationary distribution  $\rho(M)$  is calculated as the left eigenvector of  $\Pi(M) = \{\pi_{ij}(M)\}$ . As the solid green line is indistinguishable from the corresponding dashed one, ARW has always—while exploring the network—optimal spreading performances. On the contrary, by comparing the corresponding solid and dashed lines, the performances of MERW and URW are always suboptimal. In particular, MERW reaches maximum entropy production—comparable to that of ARW—only when the whole graph has been visited.

Moreover, in Fig. 1(d)–1(f) we plot the median (solid line) of the relative difference between the entropy production rate  $h$  and the optimal  $\bar{h}$ , together with first and third quartiles

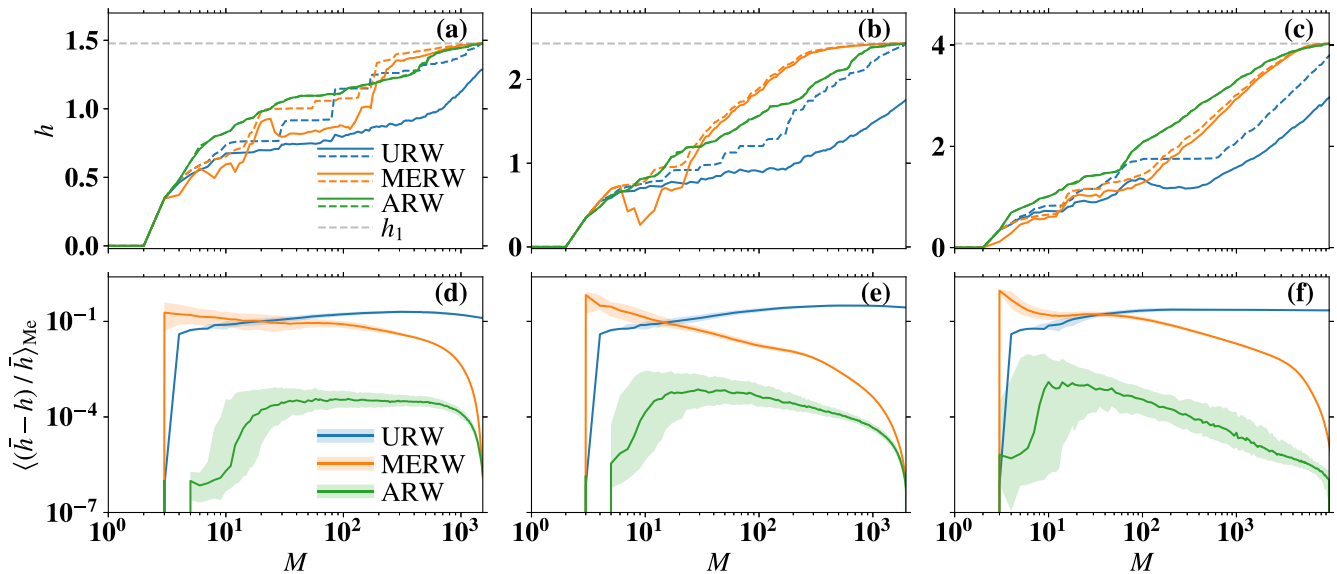


FIG. 1. [(a)–(c)] The entropy production rate  $h$ , calculated as in Eq. (16) of single trajectories of ARW, MERW and URW (solid lines) is compared to the corresponding optimal entropy production rate  $\bar{h}$  on the discovered graph (dashed lines). [(d)–(f)] Median (solid lines) and first and third quartiles (shaded area) of the normalized differences  $(\bar{h} - h)/\bar{h}$  over an ensemble of 1000 trajectories of ARW, MERW, and URW. Results are shown for random walks running on the giant connected component of an Erdős-Rényi random graph with 1000 nodes and average degree 3 in [(a), (d)], a Barabasi-Albert with 1000 nodes and  $m = 2$  [36] in [(b), (e)], and an air transportation network [57] with 3618 nodes and 14142 links in [(c), (f)].

(shaded area). The median and the quartiles are calculated over an ensemble of 1000 trajectories and are used in place of the mean and standard deviation because of the unknown distribution of  $h$  around  $\bar{h}$ . This gives further evidence of the fact that ARW performs better than MERW (and URW) at maximizing the spreading while discovering the structure of the graph. Figure S7 of the SM [63] shows the entropy production rates of ARW, MERW, and URW on the graph induced by the visited nodes, i.e., including links that have not yet been visited. In this case, ARW is still outperforming MERW and URW on the Erdős-Rényi graph, but is only marginally better on the other networks.

The optimal dispersion of the fully local ARW on the visited links of the network comes at a price: ARW takes longer than URW and MERW to cover the whole graph. This is a consequence of (i) an initial so-called warmup phase in which ARW is localised in the region where it was initialised, and (ii) a typical exploration time of the network. During the warmup phase, our process finely tunes the eigenvector centrality and the transition probability matrix to set off an efficient exploration of the network. As shown in Fig. S8 of the SM [63], where we plot the average number of time steps needed to discover new links, ARW remains indeed localised in the first few visited links. This is also the main reason why the network coverage time—the number of time steps to visit all links—is, on average,  $10^2 - 10^4$  time steps longer for ARW than for MERW or URW (see Fig. 2). We find that the coverage time  $T$  is related to the total number of links  $L$  as

$$T \propto L^\alpha, \quad (17)$$

where  $\alpha$  is the scaling exponent. Remarkably, after the initial warm up—which is evident by the overall upward shift of ARW power-law fit—the scaling exponents of ARW and

MERW are similar ( $\alpha_A \approx 2.9$ ,  $\alpha_M \approx 2.7$ ), but larger than the one of URW which has no global constraint to satisfy ( $\alpha_U \approx 1.3$ ). We remark that optimising entropy production rate and coverage time are two different tasks with the former much harder than the latter. Although having both properties is certainly appealing, our main goal is to optimize dispersion. However, in an attempt to also optimize coverage time, we point out that in our studies, the initial right eigenvector  $r_1^{(0)}$  plays a key role in determining the initial warmup time and the overall accuracy of ARW in optimizing the spreading while exploring the network (see Fig. S10 of the SM [63]). We hope that our work will stimulate further investigations to explore the tradeoff between optimal spreading accuracy and exploration times.

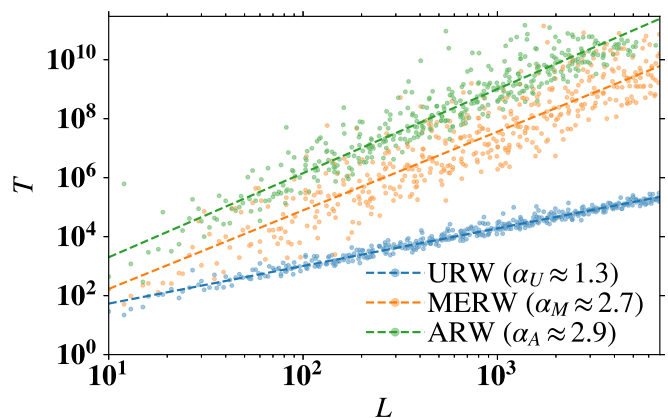


FIG. 2. Coverage time  $T$  for ARW, MERW, and URW as a function of  $L$ , i.e., the number of links in the giant connected component of Erdős-Rényi graphs with average degree 3 and increasing size.

In this Letter, we have proposed an adaptive random walk that has optimal spreading properties, outperforming the well-known MERW. Via a large-deviation tilting on the fluctuating trajectory entropy observable, ARW typically observes a maximum entropy production rate while exploring the network, exploiting only local information. Besides the theoretical novelty driven by a large-deviation study of random-walk rare events, we believe that our work can be a fundamental step towards the study of network information spreading [58,59] in all such cases where no prior knowledge on the network is available, or when the network is changing in time [37,38,60]. ARW could also be used to study dispersion properties of

other dynamical processes on real networks, e.g., aiming at optimal exploration in congested networks [61,62]. Furthermore, the algorithm at the core of ARW could also be used to sample other rare event fluctuations associated with any additive observables of random walks [39,40].

All the code used in this manuscript is available in GitHub [64].

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