

Clusters determine local fluctuations of random walks on graphs

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(Dated: October 25, 2022)

The evolution of many stochastic systems is accurately described by random walks on graphs. We here explore the close connection between local steady-state fluctuations of random walks and the global structure of the underlying graph. Fluctuations are quantified by the number of traversals of the random walk across edges during a fixed time window, more precisely, by the corresponding counting statistics. The variance-to-mean ratio of the counting statistics is typically lowered if two end vertices of an edge belong to different clusters as defined by spectral clustering. In particular, we relate the fluctuations to the algebraic connectivity and the Fiedler vector of the graph. Building on these results we suggest a centrality score based on fluctuations of random walks. Our findings imply that local fluctuations of continuous-time Markov processes on discrete state space depend strongly on the global topology of the underlying graph in addition to the specific transition rates.

I. INTRODUCTION

The representation of complex systems by graphs has been proven to be extremely useful in areas spanning physics, biology and economical sciences [1–3]. Graphs are not only suited to encode structural properties, the time evolution of many systems can be accurately modeled in terms of random walks on graphs [4, 5], for example, to investigate the performance of communication networks [6] or the motion of molecular motors on microtubules [7]. In this setting, the graph describes the discrete phase space of the system, where vertices and edges represent the states and allowed transitions, respectively. The time evolution is then equivalent to a continuous-time random walk on the graph, consisting of successive jumps between states, separated by random dwell times.

An important aspect of such models is the relation between the random walk and the underlying graph. The inevitable question is how exactly the evolution of the random walk is related to the graph topology. This question was first addressed in the work of Kirchhoff [8, 9] and much later by Hill [10, 11] and Schnakenberg [12] who related the steady-state properties of continuous-time random walks to graph elements such as spanning trees and graph cycles. The initial results have since then been considerably extended in several directions. Schnakenberg’s network theory has been applied, for instance, to classify nonequilibrium steady states [13] and to establish fluctuation theorems for nonequilibrium systems [14].

We here investigate the close connection between the local steady-state fluctuations of random walks and the

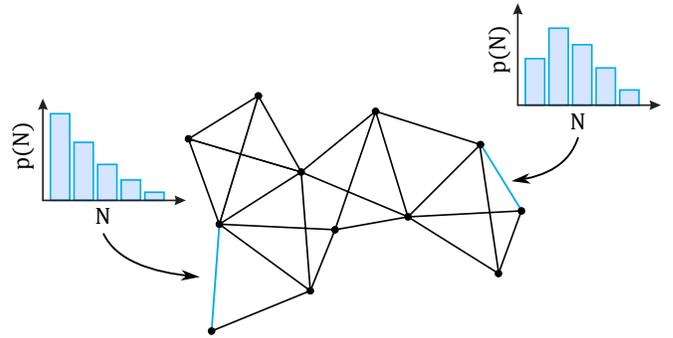


FIG. 1. The evolution of a system is modeled as a continuous-time random walk on a graph: vertices and edges represent states and allowed transitions of the system. Local steady-state fluctuations of the random walk are quantified by the counting statistics $p(N)$ of the number of jumps N across a specific edge during a fixed time window. The clusters of the underlying graph determine whether the variance-to-mean ratio of the counting statistics for an edge is either sub-Poissonian or super-Poissonian.

global structure of the underlying graph. Our practical approach to the problem mainly builds on spectral clustering theory [25] and the established tools of counting statistics [26, 27], which are used for characterizing the properties of random walks. We focus on the partition of the graph into clusters, i.e. subgraphs with highly connected vertices [28], where clusters are precisely defined by spectral clustering.

Random walks on graphs have already been exploited to define betweenness centralities [15], to characterize the similarity between vertices of graphs [16] and to detect clusters [17–20]. Specifically, centrality scores [21, 22] with the goal of identifying the most important vertices or edges of graphs are closely related to the detection of clusters [23, 24]. In contrast to our approach, however, most of these results are not based on steady-state properties of random walks.

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The local fluctuations of the random walk are specified for each edge by the number of jumps N across the edge during a fixed time window and summarized by the counting statistics for edge traversals $p(N)$, as illustrated in Fig. 1. We mainly consider the idealized case where all transition rates between states are equal to unambiguously identify the influence of the graph structure and to emphasize the role of fluctuations on top of average quantities, which in contrast are independent of the graph structure.

Our analysis allows us to establish direct relations between local fluctuations of random walks and clusters of the graph. As an example, for graphs with two dominating clusters we may write in a broad sense

$$\text{edge fluctuations} \sim \frac{\text{cluster membership}}{\text{algebraic connectivity}},$$

where the cluster membership determines the intensity of the fluctuations. If the end vertices of an edge are members of different clusters then the fluctuations are generally reduced to sub-Poissonian values.

Building on our results we put forward a new centrality score, referred to as fluctuation centrality, for identifying the most important edges of a graph, a fundamental and still unsettled problem in network analysis. The score assigns to each edge $\ell = (i, j)$ between vertices i and j the value $\sigma_{FC}(\ell) = 1/(1 + 2L_{i,j}^+)$, where L^+ is the Moore-Penrose inverse of the Laplacian matrix L . The distinguishing feature of the fluctuation centrality is that, in principle, it can be measured in physical systems that are described by random walks on graphs.

In the first part of this paper we establish the exact relation between the fluctuations of random walks and the structure of the graph and present a few basic applications. In the second part we define the fluctuation centrality score and compare it to the established betweenness centrality. Finally, we discuss possible extensions of our approach and implications of our results in the conclusions.

II. GRAPH STRUCTURE AND FLUCTUATIONS

We consider an unweighted undirected graph $G = (E, V)$ that consists of a finite set of vertices V connected by a set of edges E , where $(i, j) \in E$ denotes an edge between the vertices $i, j \in V$ and $n = |V|$ is the number of vertices. The graph is assumed to be connected and has neither multiple edges nor self-loops. Commonly used matrix representations of the graph

are the adjacency matrix A with entries

$$A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

and the Laplacian (or Kirchhoff) matrix $L = D - A$. The degree matrix D is diagonal with $D_{ii} = d_i$, where d_i is the number of edges connected to vertex i .

The eigenvalues of L form the graph spectrum, which is essential for spectral clustering. The eigenvalues are labelled such that $\lambda^{(1)} \leq \lambda^{(2)} \leq \dots \leq \lambda^{(n)}$ and $\mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \dots, \mathbf{u}^{(n)}$ are the corresponding right eigenvectors. The smallest eigenvalue $\lambda^{(1)} = 0$ is the unique zero eigenvalue with the corresponding eigenvector $\mathbf{u}^{(1)} = (1, \dots, 1)^T / \sqrt{n}$. Particularly important are the second smallest eigenvalue $\lambda^{(2)}$, known as the algebraic connectivity of G [29], and the corresponding eigenvector $\mathbf{u}^{(2)}$, called Fiedler vector [30, 31]. We assume that all right eigenvectors are normalized such that $[\mathbf{u}^{(k)}]^T \mathbf{u}^{(k)} = 1$.

The central idea of spectral clustering is that two vertices i and j belong to the same cluster if the components $u_i^{(k)}$ and $u_j^{(k)}$ of the eigenvector $\mathbf{u}^{(k)}$ have comparable values [25]. In practice, vertices are partitioned into clusters based on a small set of eigenvectors $\mathbf{u}^{(k)}$. Already the algebraic connectivity and the Fiedler vector provide substantial information about the structure of the graph. More precisely, partitioning graphs into two clusters based on the components of the Fiedler vector $\mathbf{u}^{(2)}$ is known as the spectral bisection method, i.e. two clusters are defined by vertices for which either $u_i^{(2)} \geq 0$ or $u_i^{(2)} < 0$.

A. Fluctuations of random walks

Apart from being a matrix representation, the Laplacian L is also the generator of the time evolution of the continuous-time random walk on G , restricted to the Markovian case. This type of random walk is commonly called edge-centric as opposed to vertex-centric [32]. The values of the off-diagonal entries of L are rates, all identical, for the transitions between different vertices. On the level of average quantities, the evolution is described by the occupation probabilities $w_i(t)$ that the random walk is found on vertex i at time t . The probabilities $w_i(t)$ are determined by the master equation

$$\frac{d\mathbf{w}(t)}{dt} = -L\mathbf{w}(t), \quad (2)$$

with the column vector $\mathbf{w} = (w_1, \dots, w_n)^T$. For the case of connected graphs, the eigenvector $\mathbf{u}^{(1)}$ is the

unique steady-state solution defined by the equation $L\mathbf{w}^s = 0$. The random walk in the steady state is therefore found on each vertex i with equal probability $w_i^s = 1/n$ and the occupations w_i^s are therefore independent of the graph structure.

Local fluctuations of the steady state are manifest on the level of individual trajectories, consisting of successive jumps along graph edges separated by random dwell times on vertices. To quantify local fluctuations we monitor the jumps between neighboring vertices: For an edge $\ell = (i, j) \in E$ connecting the vertices $i, j \in V$ we count the number of times N_ℓ that the random walk jumps from i to j during a fixed time window τ of sufficient length. The number of traversals N_ℓ is a random variable associated with each edge ℓ and described by the probability distribution $p_\ell(N)$, the counting statistics for transitions along graph edges.

We identify the steady-state fluctuations of the random walk at edge ℓ with the variance-to-mean ratio $\xi_\ell \equiv \text{Var}(N_\ell)/\langle N_\ell \rangle$. For a Poissonian distribution, taken as a reference here, mean and variance are equal and therefore $\xi_\ell = 1$. Deviations from the Poissonian value are referred to as sub-Poissonian $\xi_\ell < 1$ and super-Poissonian $\xi_\ell > 1$. The mean $\langle N_\ell \rangle$, similar to the occupations w_i , is identical for all edges. We will show that local fluctuations, quantified by ξ_ℓ , depend sensitively on the structure of the graph, as illustrated in Fig. 2.

Our goal is to express the variance-to-mean ratio in terms of the eigenvalues $\lambda^{(k)}$ and eigenvectors $\mathbf{u}^{(k)}$, which in turn are related to the clusters of G . To this end we follow the established theory of counting statistics [26, 27] and apply known results on parameter-dependent eigenvalues [33]. We define for each edge ℓ the modified adjacency matrix $A_\ell(\theta)$ with entries

$$[A_\ell]_{ij}(\theta) = \begin{cases} e^\theta A_{ij} & \text{if } (i, j) = \ell \\ A_{ij} & \text{otherwise} \end{cases} \quad (3)$$

and the Laplacian $L_\ell(\theta) = D - A_\ell(\theta)$, both depending on the edge ℓ and the parameter θ . The parameter-dependent matrices $A_\ell(\theta)$ and $L_\ell(\theta)$ are identical to their unmodified counterparts A and L in the limit $\theta \rightarrow 0$. We denote by $\lambda_\ell(\theta)$ the parameter-dependent eigenvalue corresponding to the zero eigenvalue $\lambda^{(1)}$ of the Laplacian, that is $\lambda_\ell(\theta) = \lambda^{(1)}$ in the limit $\theta \rightarrow 0$. The eigenvalue $\lambda_\ell(\theta)$ is related to the cumulant generating function $g_\ell(\theta) = \log \langle e^{\theta N_\ell} \rangle$ through the identity $g_\ell(\theta)/\tau = \lambda_\ell(\theta)$. All cumulants $C_{k,\ell}$ of order k of the

probability distribution $p_\ell(N)$ are found from

$$\frac{C_{k,\ell}}{\tau} = \left. \frac{\partial^k \lambda_\ell(\theta)}{\partial \theta^k} \right|_{\theta=0}. \quad (4)$$

The cumulants therefore quantify how sensitive the graph invariant $\lambda^{(1)}$ is to infinitesimally small changes in the weight of the edge ℓ .

The first two cumulants are simply the mean and variance of N_ℓ , i.e., $C_{1,\ell} = \langle N_\ell \rangle$ and $C_{2,\ell} = \text{Var}(N_\ell)$. The explicit evaluation of the derivatives of the parameter-dependent eigenvalue $\lambda_\ell(\theta)$ yields, as a main result of the paper, the mean value $\langle N_\ell \rangle = \tau/n$ and variance-to-mean ratio

$$\xi_{i,j} = 1 + 2 \sum_{k=2}^n \frac{u_i^{(k)} u_j^{(k)}}{\lambda^{(k)}} \quad \ell = (i, j). \quad (5)$$

The variance-to-mean ratio $\xi_{i,j}$ at edge $\ell = (i, j)$ is either sub- or super-Poissonian, depending on the sum on the right hand side of equation (5). If the end vertices i and j belong to the same cluster then the product $u_i^{(k)} u_j^{(k)}$ is positive. However, if vertices i and j belong to different clusters then the product can take negative values.

The situation is particularly transparent if the algebraic connectivity $\lambda^{(2)}$ is much smaller than all other eigenvalues such that

$$\xi_{i,j} \approx 1 + 2 \frac{u_i^{(2)} u_j^{(2)}}{\lambda^{(2)}} \quad \ell = (i, j). \quad (6)$$

The correction to the Poissonian variance-to-mean ratio can be substantial because the algebraic connectivity $\lambda^{(2)}$ may take small values even for large graphs [29]. This is made explicit by the general inequality $2\lambda(G)[1 - \cos(\pi/n)] \leq \lambda^{(2)} \leq \kappa(G)$, where $\lambda(G)$ and $\kappa(G)$ are the edge and vertex connectivities, respectively [34]. The product $u_i^{(2)} u_j^{(2)}$ of the components of the Fiedler vector, which partitions the graph into two dominating clusters, is negative for vertices that belong to different clusters and positive for vertices that are member of the same cluster.

It is convenient, e.g. for numerical implementations, to write equation (5) in terms of the Moore-Penrose inverse L^+ of the Laplacian matrix L [16], namely

$$\xi_{i,j} = 1 + 2L_{i,j}^+. \quad (7)$$

Both the Laplacian L and thus the matrix L^+ are symmetric and it follows immediately that for unweighted undirected graphs $\xi_{i,j} = \xi_{j,i}$.

Other interesting graph quantities such as the average first-passage time of random walks [16] and the resistance distance [35] can also be expressed in terms of the Moore-Penrose inverse. More importantly, the topological centrality [36] is closely related to the fluctuation centrality as discussed in following section. Calculating the Moore-Penrose inverse L^+ for a graph with n vertices is equivalent to finding the singular value decomposition (SVD) of the Laplacian L with a cost of $O(n^3)$ floating-point operations [37].

B. Fluctuations of Markov processes

The previous results can be further adapted to time-continuous Markov processes. For such processes the transitions are not necessarily bidirectional and characterized by specific jump rates. This can be naturally accounted for by extending the previous description to directed graphs with weighted edges. The random walk on the graph and time-continuous Markov processes are then equivalent [38].

The weighted adjacency matrix A has entries $A_{ij} = r_{ij}$ if $(i, j) \in E$ and $A_{ij} = 0$ otherwise, where r_{ij} denote the jump rates of the Markov process. The degree matrix D is diagonal with $D_{ii} = \sum_{j \neq i} r_{ij}$ and Laplacian matrix is $L = D - A$. Since the Laplacian L is not necessarily symmetric the right eigenvectors $\mathbf{u}^{(k)}$ may differ from the left eigenvectors, which are denoted by $\tilde{\mathbf{u}}^{(k)}$ and normalized such that $\tilde{\mathbf{u}}^{(k)} \mathbf{u}^{(k)} = 1$.

For the case of time-continuous Markov processes, restricted to bidirectional transitions, we then obtain the mean value

$$\langle N_\ell \rangle = \tau \tilde{u}_i^{(1)} r_{ij} u_j^{(1)} \quad \ell = (i, j) \quad (8)$$

and variance-to-mean ratio

$$\xi_{i,j} = 1 + 2 \sum_{k=2}^n \frac{\tilde{u}_i^{(k)} r_{ij} u_j^{(k)}}{\lambda^{(k)}} \quad \ell = (i, j). \quad (9)$$

The specific jump rates r_{ij} modify both the mean value $\langle N_\ell \rangle$ and the fluctuations $\xi_{i,j}$, which for random walks with equal rates are determined entirely by the graph structure. The fluctuations observed in time-continuous Markov processes are thus partly determined by the specific transition rates and partly by the graph structure of the discrete phase space.

C. Applications

We present for concreteness a few graphs and the corresponding fluctuations of the random walk. An in-

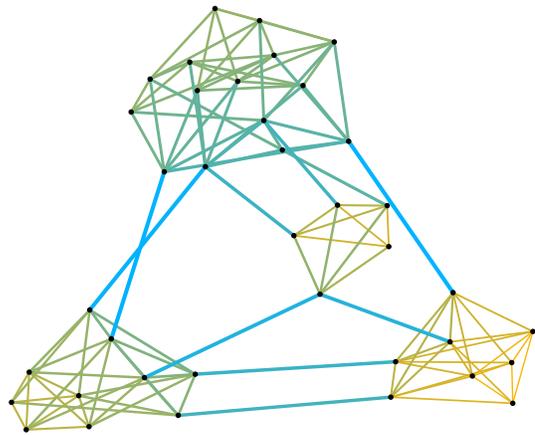


FIG. 2. A graph composed of four densely connected clusters: The steady-state fluctuations of the random walk along the bridge-like edges are sub-Poissonian whereas fluctuations within clusters are super-Poissonian, indicated by blue (thick) lines and yellow (thin) lines, respectively. The variance-to-mean ratio of the counting statistics for edge traversals ranges from 0.96 to 1.46 and the smallest four eigenvalues of the Laplacian are 0, 0.37, 0.59, 0.90.

structive example, where equation (6) is exact, is the graph consisting of two vertices connected by a single edge. The algebraic connectivity is $\lambda^{(2)} = 2$, the Fiedler vector is $\mathbf{u}^{(2)} = (-1, 1)^T / \sqrt{2}$ and the parameter-dependent eigenvalue $\lambda_\ell(\theta) = 1 + \exp(\theta/2)$. Either from equation (4) or equation (6) one finds the sub-Poissonian fluctuations $\xi_{1,2} = 1/2$.

The previous result generalizes qualitatively if the two vertices are each replaced by a cluster (cf. Fig. 3) and even if a graph is composed of several dense clusters. Let us consider several clusters that are connected by a few bridge-like edges, as exemplified by the random graph in Fig. 2. We see indeed that the fluctuations of the random walk along the bridge-like edges are reduced to sub-Poissonian values. Note that for a graph with m clusters that are only weakly connected the eigenvalues $\lambda^{(2)}, \dots, \lambda^{(m)}$ are small. As a consequence, terms weighted by the factors $1/\lambda^{(2)}, \dots, 1/\lambda^{(m)}$ contribute substantially to the sum in equation (5). Thus, only a limited set of eigenvectors is relevant for the fluctuations in strongly clustered graphs.

Random walks on highly symmetric graphs, e.g. the complete graph, star graph or cycle graph, exhibit identical fluctuations on all edges. We therefore focus on the scaling of the fluctuations with the number of vertices n . The fluctuations for a random walk on the complete graph and star graph are identical and given by $\xi_{i,j} = 1 - 2/n^2$ [39], i.e. in the limit of large graphs the fluctuations approach a Poissonian variance-to-mean ratio. In contrast, the fluctuations for the cycle graph

scale as $\xi_{i,j} = n/6 + 5/(6n)$ and therefore grow linearly with n for large graphs. Generally, these symmetric graphs have highly degenerate spectra so that none of the contributions in equation (5) can be neglected. For instance, the non-zero eigenvalues of the complete graph are all identical, namely $\lambda^{(k)} = n$ for $k \geq 2$.

III. FLUCTUATION CENTRALITY SCORE

The previous findings explicitly show that the graph structure strongly influences local fluctuations of random walks. We can therefore learn about the structural role of an edge from the observed fluctuations. A way to implement this idea is to introduce a fluctuation-based centrality score that identifies the most important edges of the graph. Such a score σ is defined as a mapping from the set of edges E (or vertices V) to the real numbers \mathbb{R} , where high scores indicate a high centrality of the edge (or vertex) [22]. Commonly used centrality measures are, for instance, the betweenness centrality [23, 24], the eigenvector centrality [40] and closeness centrality [41].

The fluctuation centrality defined here assigns to each edge ℓ the centrality score $\sigma_{FC}(\ell) = 1/\xi_\ell$ or equivalently

$$\sigma_{FC}(\ell) = \frac{1}{1 + 2L_{i,j}^+} \quad \ell = (i, j). \quad (10)$$

The fluctuation centrality is thus defined as the mean-to-variance ratio of the counting statistics for transitions along graph edges and takes positive values for all edges. Edges with a high fluctuation centrality connect different clusters, whereas a low fluctuation centrality is typical for edges within clusters. Note that alternatively any monotonically decreasing function of ξ_ℓ may be used for the definition of a fluctuation-based centrality score.

The fluctuation centrality for edges, although motivated differently, is very similar to the topological centrality for nodes, defined for node i by [36]

$$\sigma_{TC}(i) = \frac{1}{L_{i,i}^+}. \quad (11)$$

Unlike the off-diagonal elements, the diagonal elements of the Moore-Penrose inverse $L_{i,i}^+ = \sum_{k=2}^n [u_i^{(k)}]^2 / \lambda^{(k)}$ take always positive values. In the same way as the fluctuation centrality, the topological centrality of a node is a function of the entire spectrum of the Laplacian L .

Let us finally compare the fluctuation centrality to the well-known edge betweenness centrality [23, 24]. This

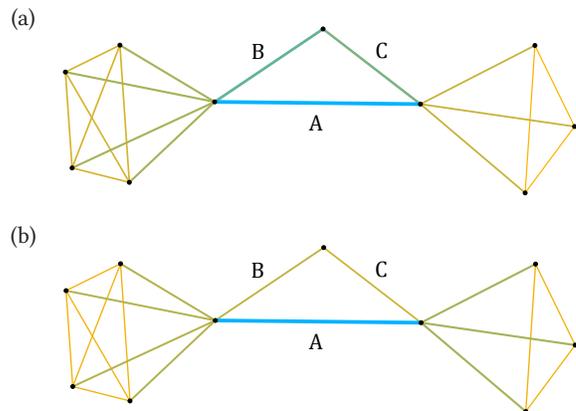


FIG. 3. The fluctuation centrality (a) in comparison to the edge betweenness (b) for two clusters connected by bridge-like edges. Blue (thick) edges correspond to high centrality and yellow (thin) edges to low centrality scores. The fluctuation centrality gives high scores to all central edges A, B and C, while the edge betweenness only singles out edge A. The scaled scores for edges A, B, C are 1.0, 0.61, 0.51 and 1.0, 0.21, 0.16 for (a) and (b), respectively.

quantity also captures the global graph structure and measures the number of shortest paths between all vertices that pass through the edge of interest. If we denote by $\gamma_{i,j}$ the number of shortest paths between vertices i and j and by $\gamma_{i,j}(\ell)$ the number of shortest paths that contain the edge ℓ then the edge betweenness is defined as

$$\sigma_{EB}(\ell) = \sum_{i,j \in V} \frac{\gamma_{i,j}(\ell)}{\gamma_{i,j}}. \quad (12)$$

An edge with a high edge betweenness $\sigma_{EB}(\ell)$ represents a central connection between different parts of a graph.

Unlike the edge betweenness, the fluctuations centrality assigns high scores to edges that are not part of a shortest path, but still act as important connectors between clusters. This is illustrated by the example of two clusters linked by a few central edges [15], shown in Fig. 3. The edge betweenness identifies edge A as most important while giving low scores to edges B and C (and all other edges). In contrast, the fluctuation centrality assigns high scores to edges A, B and C, which agrees with our intuition that all three edges are important connections between the two clusters.

The similarity to the betweenness centrality allows us to use the original Girvan-Newman algorithm [23, 24] in combination with the fluctuation centrality to detect clusters. The algorithm detects clusters by progressively removing edges such that the remaining components of the graph are highly connected. In its basic form the algorithm corresponds to finding the highest

fluctuation centralities in order to identify the two dominating clusters of the graph.

A distinguishing feature of the fluctuation centrality is the fact that, in principle, it can be measured in certain physical systems, which are described by random walks on graphs. Measuring the variance-to-mean ratio of only a few edges or even a single edge may already provide valuable information about the system. In particular, sub-Poissonian fluctuations at a single edge indicate that the edge is placed between clustered parts of the underlying graph.

IV. CONCLUSIONS

We have established a quantitative relation between steady-state fluctuations of random walks and the clusters of the underlying graph. An essential insight provided by our results is that *local* fluctuations are determined by the *global* structure of the graph, which is quantified by the fluctuation centrality score. The random walk in the steady state explores the entire graph and retrieves structural information encoded in local statistical properties.

Stochastic numerical simulation, i.e. sampling over trajectories, is an alternative and practical way to deter-

mine the fluctuations of the random walk and the fluctuation centrality score of edges. GraphStream, for example, is a Java library that allows the user to keep track of the number of edge traversals [43]. The run time of the stochastic simulation has to be significantly longer than the cover time, i.e. the expected time taken for a random walk to visit every vertex at least once [44].

Our results are relevant to Markov processes, equivalent to random walks on graphs with weighted edges. While the generalization to weighted graphs may obscure the precise role of the graph structure it covers a large class of physical systems described by classical master equations. The fluctuations in such systems thus are always determined, in principle, by both the transition rates and the structure of the discrete phase space.

The procedure presented in this paper is applicable to generators of alternative versions of random walks on graphs, either discrete or continuous in time. For any generator, the counting statistics for edge traversals is found from a parameter-dependent eigenvalue and therefore related to the eigenvectors of the generator, which in turn contain information about the structure of the graph. In particular, continuous-time *quantum* stochastic walks on graphs may reveal information that is not accessible to classical random walks [42].

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