Topologically biased random walk with application for community finding in networks

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We present a new approach of topology biased random walks for undirected networks. We focus on a one parameter family of biases and by using a formal analogy with perturbation theory in quantum mechanics we investigate the features of biased random walks. This analogy is extended through the use of parametric equations of motion (PEM) to study the features of random walks *vs.* parameter values. Furthermore, we show an analysis of the spectral gap maximum associated to the value of the second eigenvalue of the transition matrix related to the relaxation rate to the stationary state. Applications of these studies allow *ad hoc* algorithms for the exploration of complex networks and their communities.

INTRODUCTION

The study of complex networks has notably increased in the last years with applications to a variety of fields ranging from computer science[1] and biology to social science[2–4] and finance[5]. A central problem in network science [6, 7] is the study of the Random Walks (RW) on a graph, and in particular of the relation between the topological properties of the network and the properties of diffusion on it. This subject is not only interesting from a purely theoretical perspective, but it has important implications to various scientific issues ranging from epidemics [8] to the classification of web pages through PageRank algorithm [9]. Finally, RW theory is also used in algorithms for community detection [10–14].

In this paper we set up a new framework for the study of topologically biased random walks on graphs. This allows to address problems of community detection and synchronization [15] in the field of complex networks [16, 17]. In particular by using topological properties of the network to bias the RWs we explore the network structure more efficiently. A similar approach but with different focus can be found in [18]. In this research we are motivated by the idea that biased random walks can be efficiently used for community finding. To this aim we introduce a set of mathematical tools which allow us an efficient investigation of the "bias parameters" space. We apply this tools to uncover some details in the spectra of graph transition matrix, and use the relation between spectra and communities in order to introduce a novel methodology for an efficient community finding. The paper is organized as follows: in the first section we define the topologically biased random walks (TBRW). We then develop the mathematical formalism used in this paper, specifically the perturbation methods and the parametric equations of motion, to track the behaviour of different biases. In the second section we focus on the behavior of spectral gap in biased random walks. We define the conditions for which such a spectral gap is maximal and we present numerical evidence that this maximum is global. In the third section we present an invariant quantity for the biased random walk; such constant quantity depends only upon topology for a broad class of biased random walks. Finally, in the fourth section we present a general methodology for the application of different TBRW in the community finding problems. We then conclude by providing a short discussion of the material presented and by providing an outlook on different possible applications of TBRW.

BIASED RANDOM WALKS

RWs on graphs are a sub-class of Markov chains [19]. The traditional approach deals with the connection of the *unbiased* RW properties to the spectral features of *transition operators* associated to the network [20]. A generic graph can be represented by means of the adjacency matrix $\hat{\boldsymbol{A}}$ whose entries A_{ij} are 1 if an edge connects vertices i and j and 0 otherwise. Here we consider undirected graphs so that $\hat{\boldsymbol{A}}$ is symmetric. The *normal matrix* $\hat{\boldsymbol{T}}$ is related to $\hat{\boldsymbol{A}}$ through $\hat{\boldsymbol{T}} = \hat{\boldsymbol{A}}\hat{\boldsymbol{k}}^{-1}$, where $\hat{\boldsymbol{k}}$ is a diagonal matrix with $(\hat{\boldsymbol{k}})_{ii} = k_i$, i.e. the degree, or number of edges, of vertex i. In the following we use uppercase letters for non-diagonal matrices and lowercase letters for the diagonal ones. Note that by definition $k_j = \sum_i A_{ij}$. Consequently $\sum_i T_{ij} = 1$ with $T_{ij} \neq 0$ *iif* $A_{ij} = 1$, i.e. if i and j are nearest neighbors vertices. The matrix $\{T_{ij}\}$ defines the transition probabilities for an *unbiased* random walker to pass from j to i. In such a case T_{ij} has the same positive value for any of the neighbors i of j and vanishes for all the other vertices[21]. In analogy to the

operator defining the single step transition probabilities in general Markov chains, $\hat{\boldsymbol{T}}$ is also called the transition *matrix* of the unbiased RW.

A *biased* RW on a graph can be defined by a more general transition matrix $\hat{\mathbf{T}}$ where the element T_{ij} gives again the probability that a walker on the vertex j of the graph will move to the vertex i in a single step, but depending on appropriate weights for each pair of vertex (i, j). A genuine way to write these probabilities is to assign weights W_{ij} which represent the rates of jumps from vertex j to vertex i and normalize them:

$$T_{ij} = \frac{W_{ij}}{\sum_l W_{lj}}. \tag{1}$$

In this paper we consider biases which are self-consistently related to graph topological properties. For instance W_{ij} can be a function of the vertex properties (the network degree, clustering, etc.) or some functions of the edge ones (multiplicity or shortest path betweenness) or any combination of the two. There are other choices of biases found in the literature such as for instance maximal entropy related biases [22]. Some of the results mentioned in this paper hold also for biases which are not connected to graph properties as will be mentioned in any such case. Our focus on graph properties for biases is directly connected with application of biased random walks in examination of community structure in complex networks.

Let us start by considering a vertex property x_i of the vertex i (it can be either local as for example the degree, or related to the first neighbors of i as the clustering coefficient, or global as the vertex betweenness). We choose the following form for the weights:

$$W_{ij} = A_{ij}e^{\beta x_i}, \tag{2}$$

where the parameter $\beta \in \mathbb{R}$ tunes the strength of the bias. For $\beta = 0$ the unbiased case is recovered. By varying β the probability of a walker to move from vertex j to vertex i will be enhanced or reduced with respect to the unbiased case according to the property x_i of the vertex i. For instance when $x_i = k_i$, i.e. the degree of the vertex i, for positive values of the parameter β the walker will spend more time on vertices with high degree, i.e. it will be attracted by hubs. For $\beta < 0$ it will instead try to "avoid" traffic congestion by spending its time on the vertices with small degree. The entries of the transition matrix can now be written as:

$$T_{ij}(\boldsymbol{x}, \beta) = \frac{A_{ij}e^{\beta x_i}}{\sum_l A_{lj}e^{\beta x_l}} \equiv \frac{A_{ij}e^{\beta x_i}}{z_j(\beta)}. \tag{3}$$

For this choice of bias we find the following results: (i) we have a unique representation of any given network via operator $\hat{\boldsymbol{T}}(\boldsymbol{x}, \beta)$, i.e. knowing the operator, we can reconstruct the graph; (ii) for small $|\beta|$ we can use perturbation methods around the unbiased case; (iii) this choice

of bias permits in general also to visit vertices with vanishing feature x, which instead is forbidden for instance for a power law $W \sim x^\alpha$; (iv) this choice of biases is very common in the studies of energy landscapes, when biases represent energies $x_i \equiv E_i$ (see for example [23] and references therein).

In a similar way one can consider a *symmetric* edge property y_{ij} (for instance edge multiplicity or shortest path betweenness) as bias. In this case we can write the transition probability as:

$$T_{ij}(\hat{\boldsymbol{Y}}, \beta) = \frac{A_{ij}e^{\beta y_{ij}}}{\sum_l A_{lj}e^{\beta y_{lj}}}. \tag{4}$$

The general case of some complicated multiparameter bias strategy can be finally written as

$$T_{ij}(\boldsymbol{x}, \hat{\boldsymbol{Y}}, \boldsymbol{\beta}) = \frac{A_{ij}e^{\sum_\nu \beta_\nu x_i^{(\nu)} + \sum_\mu \beta_\mu y_{ij}^{(\mu)}}}{\sum_l A_{lj}e^{\sum_\nu \beta_\nu x_l^{(\nu)} + \sum_\mu \beta_\mu y_{lj}^{(\mu)}}}. \tag{5}$$

While we mostly consider biased RW based on vertex properties, as shown below, most of the results can be extended to the other cases. The transition matrix in the former case can also be written as: $\hat{\boldsymbol{T}}(x, \beta) = \hat{\boldsymbol{w}}\hat{\boldsymbol{A}}\hat{\boldsymbol{z}}^{-1}$, where the diagonal matrices $\hat{\boldsymbol{w}}$ and $\hat{\boldsymbol{z}}$ are such that $w_{ii} = e^{\beta x_i}$ and $z_{ii}^{-1} = 1/\sum_l A_{li}e^{\beta x_l}$. The Frobenius-Perron theorem implies that the largest eigenvalue of $\hat{\boldsymbol{T}}(x, \beta)$ is always $\lambda_1(\beta) = 1$ [19]. Furthermore, the eigenvector $\boldsymbol{v}_1$ associated to λ_1 is strictly positive in a connected aperiodic graph. Its normalized version, denoted as $\boldsymbol{p}(\beta)$, gives the asymptotic stationary distribution of the biased RW on the graph. Assuming for it the form $p_i(\beta) = \Omega(\beta)^{-1}g_i(\beta)z_i(\beta)$, where $z_i = \sum_j A_{ij}e^{\beta x_j}$ and $\Omega(\beta) > 0$ is a normalization constant, and plugging this in the equation $\boldsymbol{p} = \hat{\boldsymbol{T}}\boldsymbol{p}$ we get:

$$\begin{aligned} p_i &= \sum_j T_{ij}(\boldsymbol{x}, \beta)p_j \\ &= \Omega^{-1}e^{\beta x_i}\sum_j A_{ij}g_j. \end{aligned} \tag{6}$$

Hence the equation holds *iif* $g_i = e^{\beta x_i}$. Therefore the stable asymptotic distribution of vertex centerd biased RWs is

$$p_i(\beta) = \Omega(\beta)^{-1}e^{\beta x_i}z_i(\beta). \tag{7}$$

For $\beta = 0$ we have the usual form of the stationary distribution in an unbiased RW where $z_i(0) = k_i$ and $\Omega(0) = \sum_i k_i$. For general β it can be easily demonstrated that the asymptotic solution of edge biased RW is $p_i = \Omega^{-1}z_i$, while for multiparametric RW the solution is $p_i = \Omega^{-1}e^{\sum_\nu \beta_\nu x_i^{(\nu)}}z_i$.

Using Eqs. (7) and (3) we can prove that the detailed balance condition $T_{ij}p_j = T_{ji}p_i$ holds.

At this point it is convenient to introduce a different approach to the problem [10]. We start by symmetrizing the matrix $\hat{\boldsymbol{T}}(\boldsymbol{x},\beta)$ in the following way:

$$\hat{\boldsymbol{T}}^{s}(\boldsymbol{x},\beta) = [\hat{\boldsymbol{p}}(\beta)]^{-1/2}\hat{\boldsymbol{T}}(\boldsymbol{x},\beta)[\hat{\boldsymbol{p}}(\beta)]^{1/2}, \qquad (8)$$

where $\hat{\boldsymbol{p}}(\beta)$ is the diagonal matrix with the stationary distribution $\{p_i(\beta)\}$ on the diagonal. The entries of the symmetric matrix for vertex centered case are given by

$$T_{ij}^{s}(\boldsymbol{x},\beta) = T_{ji}^{s}(\boldsymbol{x},\beta) = A_{ij}\frac{e^{\frac{1}{2}\beta(x_i+x_j)}}{\sqrt{z_i z_j}}. \qquad (9)$$

The symmetric matrix $\hat{\boldsymbol{T}}^{s}(\boldsymbol{x},\beta)$ shares the same eigenvalues with the matrix $\hat{\boldsymbol{T}}(\boldsymbol{x},\beta)$; anyhow the set of eigenvectors is different and forms a complete orthogonal basis, allowing to define a meaningful "distance" between vertices. Such distance can provide important additional information in the problem of community partition of complex networks. If $\mathbf{v}_\nu$ is the νth eigenvector of the asymmetric matrix $\hat{\boldsymbol{T}}(\boldsymbol{x},\beta)$ associated to the eigenvalue $\lambda_\nu(\beta)$ (therefore $\mathbf{v}_1 = \mathbf{p}$), the corresponding eigenvector $|v_\nu\rangle$ of the symmetric matrix $\hat{\boldsymbol{T}}^{s}(\boldsymbol{x},\beta)$, can always be written as $|v_\nu\rangle_i = \frac{v_{\nu,i}}{\sqrt{p_i}}$. In particular for $\nu=1$ we have $|v_1\rangle_i \equiv |p\rangle_i = \sqrt{p_i}$. The same transformation (8) can be applied to the most general multiparametric RW. In that case the symmetric operator is

$$T_{ij}^{s}(\boldsymbol{x},\beta) = T_{ji}^{s}(\boldsymbol{x},\beta) = A_{ij}\frac{e^{(\sum_\nu \frac{\beta_\nu}{2}(x_i^{(\nu)}+x_j^{(\nu)})+\sum_\mu \beta_\mu y_{ij}^{(\mu)})}}{\sqrt{z_i z_j}}. \qquad (10)$$

This form also enables usage of perturbation theory for Hermitian linear operators. For instance, knowing the eigenvalue $\lambda_\nu(\beta)$ associated to eigenvector $|v_\nu(\beta)\rangle$, we can write the following expansions at sufficiently small $\Delta\beta$: $\lambda_\nu(\beta+\Delta\beta) = \lambda_\nu(\beta) + \Delta\beta\lambda_\nu^{(1)}(\beta) + \ldots$ and $|v_\nu(\beta+\Delta\beta)\rangle = |v_\nu^{(0)}(\beta)\rangle + \Delta\beta|v_\nu^{(1)}(\beta)\rangle + \ldots$. It follows that for a vertex centered bias

$$\lambda_\nu^{(1)}(\beta) = \langle v_\nu(\beta)|\hat{\boldsymbol{T}}^{s(1)}(\boldsymbol{x},\beta)|v_\nu(\beta)\rangle, \qquad (11)$$

where,

$$\hat{\boldsymbol{T}}^{s(1)}(\boldsymbol{x},\beta) \equiv \frac{\partial \hat{\boldsymbol{T}}^{s}(\boldsymbol{x},\beta)}{\partial\beta} = \frac{1}{2}\left[\{\hat{\boldsymbol{x}},\hat{\boldsymbol{T}}^{s}\}_+ - \{\hat{\bar{\boldsymbol{x}}}(\beta),\hat{\boldsymbol{T}}^{s}\}_+\right] \qquad (12)$$

with $\{\cdot,\cdot\}_+$ being the anticommutator operator. Operator $\hat{\boldsymbol{x}}$ and $\hat{\bar{\boldsymbol{x}}}(\beta)$ are diagonal matrices with $(\hat{\boldsymbol{x}})_{ii} = x_i$ and $\hat{\bar{\boldsymbol{x}}}_{ii}(\beta) = \sum_l A_{li}x_l e^{\beta x_l}/z(i)$ which is the expected value of x that an random walker, will find moving from vertex i to its neighbors. In the case of edge bias the change of symmetric matrix with parameter β can be written as $\frac{\partial \hat{\boldsymbol{T}}^{s}(\beta)}{\partial\beta} = \hat{\boldsymbol{Y}} \star \hat{\boldsymbol{T}}^{s}(\beta) - 1/2\{\hat{\bar{\boldsymbol{y}}},\hat{\boldsymbol{T}}^{s}(\beta)\}_+$, and $\star$ represents the Schur-Hadamard product i.e. element wise multiplication of matrix elements. The eigenvector components

in $\beta+\Delta\beta$ at the first order of expansion in the basis of the eigenvectors at β are given by (for $\mu \neq \nu$):

$$\langle v_\mu(\beta)|v_\nu^{(1)}(\beta)\rangle = \frac{\langle v_\mu(\beta)|\hat{\boldsymbol{T}}^{s(1)}(\beta)|v_\nu(\beta)\rangle}{\lambda_\mu(\beta) - \lambda_\nu(\beta)}. \qquad (13)$$

For $\mu = \nu$ the product $\langle v_\mu(\beta)|v_\nu^{(1)}(\beta)\rangle$ vanishes and eqs. (12) and (13) hold only for non-degenerate cases. In general, usual quantum mechanical perturbation theory can be used to go to higher order perturbations or to take into account degeneracy of eigenvalues.

We can also exploit further the formal analogy with quantum mechanics using Parametric Equations of Motion (PEM) [24, 25] to study the β dependence of the spectrum of $\hat{\boldsymbol{T}}^{s}$. If we know such spectrum for one value of β, we can calculate it for any other value of β by solving a set of differential equations corresponding to PEM in quantum mechanics. They are nothing else the expressions of Eqs. (11) and (13) in an arbitrary complete orthonormal base $\{|\phi_\nu\rangle\}$. First the eigenvector is expanded in such a base: $|v_\nu(\beta)\rangle = \sum |\phi_\xi\rangle\langle\phi_\xi|v_\nu(\beta)\rangle \equiv \sum_\xi c_{\nu\xi}(\beta)|\phi_\xi\rangle$. We can then write

$$\frac{\partial\lambda_\nu}{\partial\beta} = \boldsymbol{c}_\nu^{\mathsf{T}}(\beta)\frac{\partial\hat{\boldsymbol{T}}^{s,\phi}(\beta)}{\partial\beta}\boldsymbol{c}_\nu(\beta), \qquad (14)$$

where $\boldsymbol{c}_\nu$ ($\boldsymbol{c}_\nu^{\mathsf{T}}$) is a column (row) vector with entries $c_{\nu\xi}(\beta)$ and $\hat{\boldsymbol{T}}^{s,\phi}$ is the matrix with entries $\hat{T}_{\nu\xi}^{s,\phi}(\beta) \equiv \langle\phi_\nu|\hat{\boldsymbol{T}}^{s}(\beta)|\phi_\xi\rangle$. Let us now define the matrix $\hat{\boldsymbol{N}}(\beta)$ whose rows are the copies of vector $\boldsymbol{c}_\nu^{\mathsf{T}}(\beta)$. The differential equation for the eigenvectors in the basis $\{|\phi_\nu\rangle\}$ is then [25]

$$\frac{\partial\boldsymbol{c}_\nu(\beta)}{\partial\beta} = \left(\hat{\boldsymbol{T}}^{s,\phi}(\beta) - \lambda_\nu(\beta) + \hat{\boldsymbol{N}}(\beta)\right)^{-1} \cdot$$
$$\left(\boldsymbol{c}_\nu^{\mathsf{T}}(\beta)\frac{\partial\hat{\boldsymbol{T}}^{s,\phi}(\beta)}{\partial\beta}\boldsymbol{c}_\nu(\beta) - \frac{\partial\hat{\boldsymbol{T}}^{s,\phi}(\beta)}{\partial\beta}\right)\boldsymbol{c}_\nu(\beta). \qquad (15)$$

A practical way to integrate Eqs. (14) and (15) can be found in [25]. In order to calculate parameter dependence of eigenvectors and eigenvalues, the best way to proceed is to perform an LU decomposition of the matrix $\left(\hat{\boldsymbol{T}}^{s,\phi}(\beta) - \lambda_\nu(\beta) + \hat{\boldsymbol{N}}(\beta)\right)^{-1}$ as the product of a lower triangular matrix $\hat{\boldsymbol{L}}$ and an upper triangular matrix $\hat{\boldsymbol{U}}$, and integrate differential equations of higher order which can be constructed in the same way as equations (14) and (15) [25]. A suitable choice for the basis is just the ordinary unit vectors spanned by vertices, i.e. $\{|\phi\rangle\} \equiv \{|e\rangle\}$. We found that for practical purposes, depending on the studied network, it is appropriate to use PEM until the error increases to much and then diagonalize matrix again to get better precision. PEM efficiently enables study of the large set of parameters for large networks due to its compatitive advantage over ordinary diagonalization.
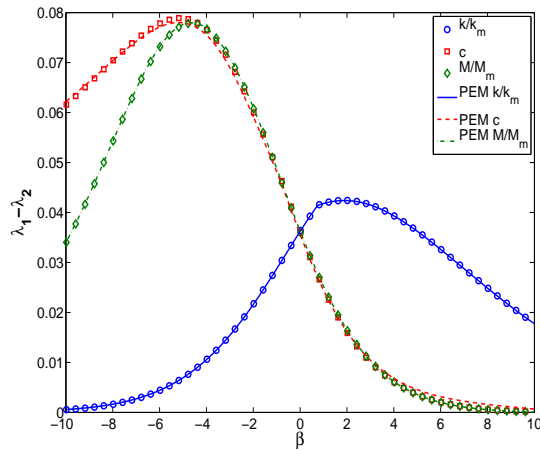
FIG. 1: (color on line) Plot of the spectral gap $\lambda_1 - \lambda_2$ vs β for networks of 10 communities with 10 vertices each (the probability for an edge to be in a community is $p_i = 0.3$ while outside of the community it is $p_o = 0.05$). Solid points represent the solutions computed via diagonalization, while lines report the value obtained through integration of PEM. Different bias choice have been tested. Circles (blue) are related to degree-based strategy, square (red) are related to clustering-based strategies, diamonds (green) multiplicity-based strategies. The physical quantities to get the variable x in Eq. (2) in these strategies have been normalized with respect to their maximum value.

SPECTRAL GAP

A key variable in the spectral theory of graphs is the *spectral gap* $\mu = (\lambda_1 - \lambda_2)$, i.e. the difference between first unitary and the second eigenvalues. The spectral gap measures how fast the information on the RW initial distribution is destroyed and the stationary distribution is approached. The characteristic time for that is $\tau = -1/\ln[(1 - \mu)] \simeq 1/\mu$ [10]. We show in Fig. 1 the dependence of spectral gap of simulated graphs with communities for different strategies (degree, clustering and multiplicity based) at a given value of parameter β. In all investigated cases the spectral gap has its well defined maximum, i.e. the value of parameter β for which the random walker converges to stationary distribution with the largest rate.

The condition of maximal spectral gap implies that it is a stationary point for the function $\lambda_2(\beta)$, i.e. that its first order perturbation coefficient vanishes at this point:

$$\begin{aligned}
0 &= \langle v_2(\beta_m) | \frac{\partial \hat{\boldsymbol{T}}^s(\beta_m)}{\partial \beta} | v_2(\beta_m) \rangle \\
&= \langle v_2(\beta_m) | \left[\hat{\boldsymbol{x}} - \hat{\bar{\boldsymbol{x}}}(\beta_m) \right] | v_2(\beta_m) \rangle,
\end{aligned} \tag{16}$$

where $\hat{\boldsymbol{x}}$ and $\hat{\bar{\boldsymbol{x}}}$ are defined above. The squares of entries $c_{2,i}^2(\beta)$ of the vector $|v_2(\beta)\rangle$ in the chosen basis $|\phi_i\rangle \equiv |e\rangle$, define a particular measure on the graph. Equation (16) can be written as

$\sum_i c_{2,i}^2(\beta_m)(x_i - \bar{x}_i(\beta_m)) = 0$. Thus we conclude that the local spectral maximum is achieved if the average difference between property x_i and its expectation $\bar{x}_i$, with respect to this measure, in the neighborhood of vertex i vanishes. We have studied behavior of spectral gap for different sets of real and simulated networks (Barabási-Albert model with different range of parameters, Erdős-Rényi model and random netwroks with given community structure) and three different strategies (degree-based, clustering-based and multiplicity-based). Although in general it is not clear that the local maximum of spectral gap is unique, we have found only one maximum in all the studied networks. This observation is interesting because for all cases the shapes of spectral gap *vs.* β looks typically Gaussian-like. In both limits $\beta \to \pm\infty$ the spectral gap of heterogeneous network is indeed typically zero, as the RW stays in the vicinity of the vertices with maximal or minimal value of studied property x_i.

RANDOM WALK INVARIANT

A fundamental question in the theory of complex networks is how topology affects dynamics on networks. Our choice of β-parametrized biases provides a useful tool to investigate this relationship. A central issue is, for instance, given by the search of properties of the transition matrix $\boldsymbol{T}$ which are independent of β and the chosen bias, but depend only on the topology of the network. An important example comes from the analysis the determinant of $\boldsymbol{T}$ as a function of the bias parameters:

$$\frac{\partial \prod_{\mu=1}^{N} \lambda_\mu}{\partial \beta} = \sum_{\mu=1}^{N} \langle \mu | \frac{\partial \boldsymbol{T}^s}{\partial \beta} | \mu \rangle \prod_{\nu \neq \mu} \lambda_\nu, \tag{17}$$

For vertex centered bias using eq. (12) we have

$$\frac{\partial \prod_{\mu=1}^{N} \lambda_\mu}{\partial \beta} = \sum_{\mu=1}^{N} \langle \mu | (\hat{\boldsymbol{x}} - \hat{\bar{\boldsymbol{x}}} | \mu \rangle \prod_{\nu=1}^{N} \lambda_\nu. \tag{18}$$

and using the diagonality of the $\hat{\boldsymbol{x}}$ and $\hat{\bar{\boldsymbol{x}}}_{ii}(\beta) = \frac{\partial \ln z_i}{\partial \beta}$

$$\prod_{\mu=1}^{N} \frac{\lambda_\mu(\beta) z_\mu(\beta)}{e^{\beta x_\mu}} = \prod_{\mu=1}^{N} \frac{\lambda_\mu(\beta_0) z_\mu(\beta_0)}{e^{\beta_0 x_\mu}}. \tag{19}$$

In other words the quantity $\prod_{\mu=1}^{N} \frac{\lambda_\mu(\beta) z_\mu(\beta)}{e^{\beta x_\mu}}$ is a topological constant which does not depend on the choice of parameters. For $\beta = 0$ we get $\prod_{\mu=1}^{N} \lambda_\mu k_\mu = const$ and it follows that this quantity does not depend on the choice of vertex biases x_i either. It can be shown that such quantity coincides with the determinant of adjacency matrix which must be conserved for all processes.
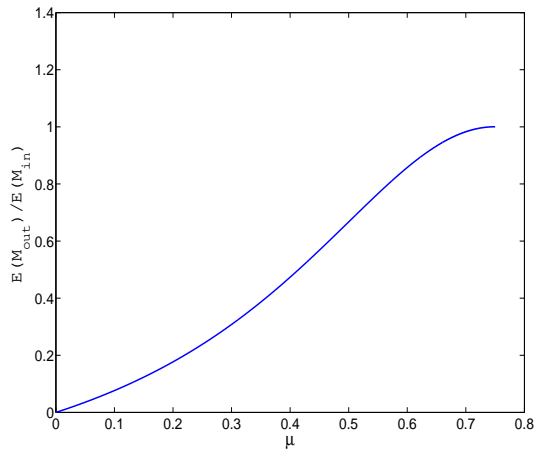
FIG. 2: (color on line) The ratio between expected value of multiplicity for edges that are connecting vertices in different communities to the expected value of multiplicity for edges that are connecting vertices in the same community with respect to parameter μ.
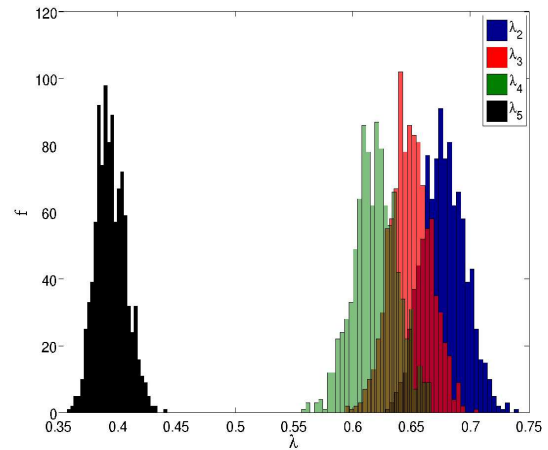

FIG. 3: (color on line) Histogram of second, third, fourth and fifth eigenvalue of non-biased RW for 1000 GN networks with parameters $N = 128$, $n = 32$, $p_{in} = 0.35$, $p_{out} = 0.05$. There is a clear gap between "community" band and the rest of the eigenvalues.

COMMUNITY FINDING

There are many competing algorithms and methods for community detection [26]. Despite a significant scientific effort to find such reliable algorithms, there is not yet agreement on a single general solving algorithm for the various cases. In this section instead of adding another precise recipe, we want to suggest a general methodology based on TBRW which could be used for community detection algorithms. To add trouble, the very definition of communities is not a solid one. In most of the cases we define communities as connected subgraphs whose density of edges is larger within the proposed community than outside it (a concept quantified by modularity [14]).

Scientific community is therefore thriving to find a benchmark in order to assess the success of various methods. One approach is to create synthetic graphs with assigned community structure (benchmark algorithms) and test through them the community detection recipes [27]. The Girvan-Newman (GN) [14] and Lancichinetti-Fortunato-Radicchi (LFR) [28, 29] are the most common benchmark algorithms. In both these models several topological properties (not only edge density) are unevenly distributed within the same community and between different ones. We use this property to propose a novel methodology creating suitable TBRW for community detection. The difference between internal and external part of a community is related to the "physical" meaning of the graph. In many real processes the establishment of a community is facilitated by the subgraph structure. For instance in social networks agents have a higher probability of communication when they share a lot of friends. We test our approach on GN benchmark since in this case we can easily compute the expected differences between the frequency of biased variables within and outside the community.

In this section we will describe how to use TBRW for community detection. For $\beta = 0$ our method is rather similar to the one introduced by Donetti and Muñoz [30]. The most notable difference is that we consider the spectral properties of transition matrix instead of the Laplacian one. We decide if a vertex belongs to a community according to the following ideas: (i) We expect that the vertices belonging to the same community to have similar values of eigenvectors components; (ii) we expect relevant eigenvectors to have the largest eigenvalues. Indeed, spectral gap is associated with temporal convergence of random walker fluctuations to the ergodic stationary state. If the network has well defined communities, we expect the random walker to spend some time in the community rather than escaping immediately out of it. Therefore the speed of convergence to the ergodic state should be related to the community structure. Therefore eigenvectors associated with largest eigenvalues (except for the maximal eigenvalue 1) should be correlated with community structure. Coming back to the above mentioned Donetti and Muñoz approach here we use the fact that some vertex properties will be more common inside a community and less frequent between different communities. We then vary the bias parameters trying both to shrink the spectral gap in transition matrix and to maximize the separation between relevant eigenvalues and the rest of the spectra.

For example in the case of GN benchmark the network consist of 4 communities each with $n = 32$ vertices i.e.
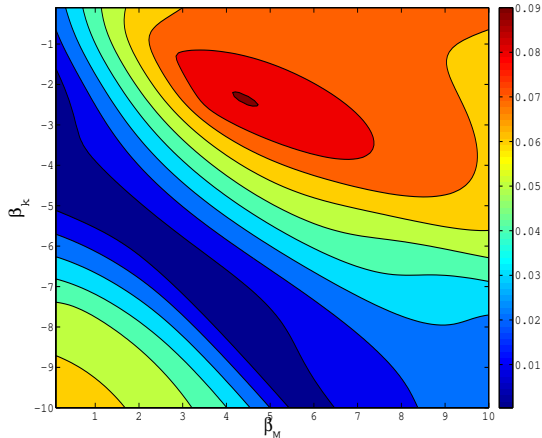
FIG. 4: (color on line) Contour plot of the difference between fourth and fifth eigenvalue $\lambda_4 - \lambda_5$ as a function of parameter β_k which biases RW according to degrees of the vertices and parameter β_M which bias RW according to multiplicities of the edges. Both degrees and multiplicity values are normalized with respect to the maximal degree and multiplicity (therefore the largest value is one).

$N = 128$ vertices all together. The probability that the two vertices which belong to the same community are connected is p_{in}. The probability that the two vertices which belong to different communities are connected is p_{out}. The fundamental parameter [26] which characterizes the difficulty of detecting the structure is

$$\mu = \frac{\bar{k}_{out}}{\bar{k}_{out} + \bar{k}_{in}}, \tag{20}$$

where $\bar{k}_{out} = p_{out}(N - n)$ is the mean degree related to inter-community connections and $\bar{k}_{in} = p_{in}(n - 1)$ is the mean degree related to edges inside-community. As a rule of thumb we can expect to find well defined communities when $\mu < 1/2$, and observe some signature of communities even when $\mu < 3/4$ [27]. The probabilities p_{in} and p_{out} are related via the control parameter μ as $p_{out} = \frac{(n-1)\mu}{(N-n)(1-\mu)}p_{in}$.

We now examine the edge multiplicity. The latter is defined as the number of common neighbors shared by neighbouring vertices. The expected multiplicity of an edge connecting vertices inter-community and inside-communities are respectively

$$\begin{aligned} E(M_{out}) &= 2p_{in}p_{out}(n-1) + p_{out}^2(N - 2n), \\ E(M_{in}) &= p_{in}^2(n-2) + p_{out}^2(N-n) \end{aligned} \tag{21}$$

On Fig. 2 we plot the ratio of the quantitites above defined, $E(M_{out})/E(M_{in})$, vs. the parameter μ.

We see that even for $\mu > 0.5$ the ratio remains smaller than 1 implying that the multiplicity is more common in the edges in the same community. Based on this analysis for this particular example we expect that if we want

to find well-defined communities via TBRW we have to increase bias with respect to the multiplicity. Through numerical simulations we find that the number of communities is related to number of eigenvalues in the "community band". Namely one in general observes a gap between eigenvalues $\lambda_2, ..., \lambda_{N/n-1}$ and the next eigenvalue evident in a network with a strong community structure ($\mu \ll 1/2$). The explanation that we give for that phenomenon can be expressed by considering a network of n separated graphs. For such a network there are n degenerate eigenvalues $\lambda_1 \dots \lambda_n = 1$. If we now start to connect these graphs with very few edges such a degeneracy is broken with the largest eigenvalue remaining 1 while the next $(n-1)$ eigenvalues staying close to it. The distance between any two of this set of $(n-1)$ eigenvalues will be smaller than the gap between this community band and the rest of the eigenvalues in the spectrum. Therefore, the number of eigenvalues different of 1 which are forming this "community band" is always equal to the number of communities minus one, at least for different GN-type networks with different number of communities and different sizes, as long as $\mu \ll 1/2$. For example in the case of 1000 GN networks described with parameters $N = 128$, $n = 32$, $p_{in} = 0.35$, $p_{out} = 0.05$, i.e. $\mu = 0.125$, the histograms of eigenvalues are depicted on figure 3.

For our purposes we used two parameters biased RW, in which topological properties are $x_i \equiv k_i/max(k)$ i.e. the normalized degree (with respect to maximal degree in the network) and $y_{ij} = M_{ij}/max(M_{ij})$ i.e. the normalized multiplicity (with respect to maximal multiplicity in the network). We choosed GN network whose parameters are $N = 128$, $n = 32$, $p_{in} = 16/62$ and $p_{out} = 1/12$, for which $\mu = 1/2$. Being $N/n = 4$ the number of communities, as a criterion for good choice of parameters we decided to use the difference between λ_4 and λ_5, i.e., we decided to maximize the gap between "community band" and the rest of eigenvalues; checking at the same time that the spectral gap shrinks. In Fig. 4, we plot such a quantity with respect to different biases.

It is important to mention that for every single network instance there are different optimal parameters. This can be seen on figure 5, where we show the difference between unbiased and biased eigenvalues for 1000 GN nets created with same parameters. As shown in the figure the difference between fourth and fifth eigenvalue is now not necessarily the optimal for this choice of parameters. Every realization of the network should be independently analyzed and its own parameters should be carefully chosen. In the Figs. 6 and 7 we present instead the difference between unbiased and biased projection on three eigenvectors with largest nontrivial eigenvalues. Using 3D view it is easy to check that communities are better separated in the biased case then in the non-biased case.
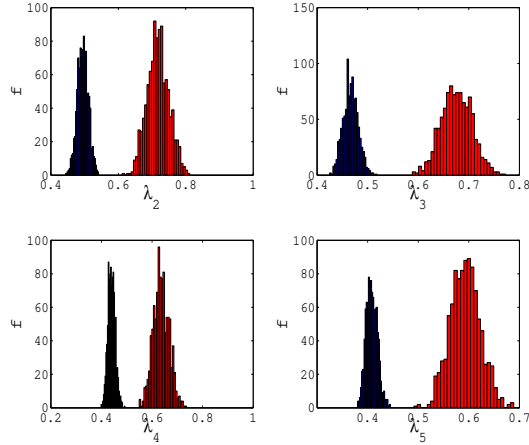
FIG. 5: (color on line) Histograms of λ_2, λ_3, λ_4 and λ_5 for 1000 GN networks described with parameters $N = 128$, $n = 32$, $p_{in} = 16/62$ and $p_{out} = 1/12$. With black colour we indicate the eigenvalues of nonbiased RW, while with red we indicate the eigenvalues of RW biased with parameters $\beta_k = -2.5$ and $\beta_M = 4.3$. Note how this choice of parameters does not maximize "community gap" for all the different realizations of monitored GN network.

FIG. 7: (color on line) Plot of the eigenvector components of the second, third and fourth eigenvector of biased RW with parameters $\beta_k = -2.5$ and $\beta_M = 4.3$. Different markers represent four different predefined communities. This is an example of the same GN graph realization with $p_{in} = 16/62$ and $p_{out} = 1/12$ as the one on the previous figure. For this choice of parameters $\mu = 1/2$. One can notice tetrahedral distribution of vertices in which vertices from the same community belong to the same branch of tetrahedron.
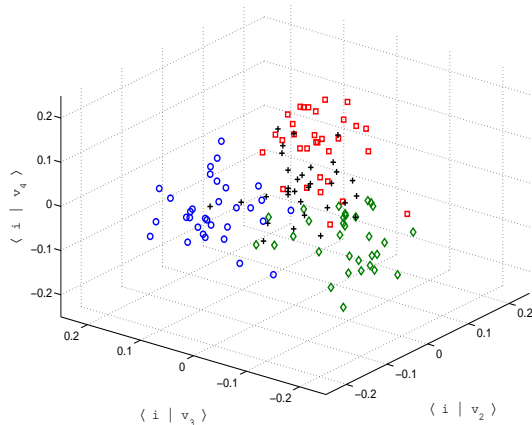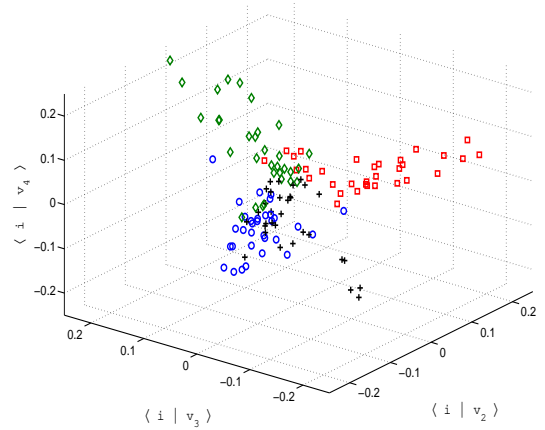

FIG. 6: (color on line) Plot of the eigenvector components of the second, third and fourth eigenvector. Different markers represent four different predefined communities. This is an example of GN graph with $p_{in} = 16/62$ and $p_{out} = 1/12$. For this choice of parameters $\mu = 1/2$. There is a strong dispersion between different vertices which belong to the same community.

CONCLUSION

In this paper we presented a detailed theoretical framework to analyze the evolution of TBRW on a graph. By using as bias some topological property of the graph itself allows to use the RW as a tool to explore the environment. This method maps vertices of the graph to dif-

ferent points in the N-dimensional Euclidean space naturally associated with the given graph. In this way we can measure distances between vertices depending on the chosen bias strategy and bias parameters. In particular we developed a perturbative approach to the spectrum of eigenvalues and eigenvectors associated with the transition matrix of the system. More generally we generalized the quantum PEM approach to the present case. This led naturally to study the behavior of the gap between the largest and the second eigenvalue of the spectrum characterizing the relaxation to the stationary Markov state. In numerical applications of such a theoretical framework we have observed a unimodal shape of the spectral gap *vs.* the bias parameter which is not an obvious feature of the studied processes. We have finally outlined a very promising application of topologically biased random walks to the fundamental problem of community finding. We described the basic ideas and proposed some criteria for the choice of parameters, by considering the particular case of GN graphs. We are working further in direction of this application, but the number of possible strategies (different topological properties we can use for biasing) and types of networks is just too large to be presented in one paper. Furthermore, since in many dynamical systems as the WWW or biological networks, a feedback between function and form (topology) is evident, our framework may be a useful way to describe mathematically such an observed mechanism. In the case of biology, for instance, the shape of the metabolic networks can be triggered not only by the chemical proper-

ties of the compounds, but also by the possibility of the metabolites to interact. Biased RW can be therefore the mechanism through which a network attains a particular form for a given function. By introducing such approach we can now address the problem of community detection in the graph. This the reason why here we have not introduced another precise method for community detection, but rather a possible framework to create different community finding methods with different *ad hoc* strategies. Indeed in real situations we expect different types of network to be efficiently explored by use of different topological properties. This explains why we believe that TBRW could play a role in community detection problems, and we hope to stimulate further developments, in the network scientific community, of this promising methodology.

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