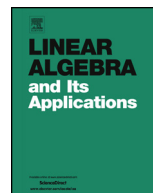




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Random walks associated with symmetric M -matrices

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ABSTRACT

In this paper we generalize the transition probability matrix for a random walk on a finite network by defining the transition probabilities through a symmetric M -matrix. Usually, the walker jumps from a vertex to a neighbor according to the probabilities given by the adjacency matrix. Moreover, we can find in the literature the relation between random walks and the normalized laplacian or the combinatorial laplacian that are singular and symmetric M -matrices. Our model takes into consideration not only the probability of transitioning given by the adjacency matrix but also some added probability that depends on a node property. This also includes the probability of remaining in each node, when the M -matrix is not singular. The nodes importance is taking into account by considering the lower eigenvalue and its associated eigenfunction for the given M -matrix. We give expressions for the mean first passage time and Kemeny's constant for such a random walks in terms of 1-inverses of the considered M -matrix.

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1. Introduction

All the standard models in random walks are based on the hypothesis that in each step the walker moves from one node to another different one. Only the so-called lazy random walks contemplate the probability of remaining at a state, but this probability is always constant and usually equal to $1/2$, see [8]. Therefore, they are far away to include all the real situations that would be modeled in this context. Assigning a different positive transition probability to each node will include the probability to remain in each state, depending on the state, and suppose a challenge in random walks theory. In addition, by doing that we are also adding a new arbitrary probability of reaching a node. The latter is what the so-called biased random walks do [11,17], but without considering the possibility of remaining in a node and, furthermore, fixing the value of each of the new probabilities assigned to the nodes that respond to a certain property of them. Moreover, in our model the lazy term can be considered as a function instead of a parameter.

Our experience in the study of discrete potential theory, and in particular of M -matrices [3], will allow us to consider a generalization of random walks that have importance in applications where it is necessary taking into account the possible different properties of each node of the network that model the random walk. To achieve that, we must incorporate M -matrices into the analysis of random walks. When we consider a transition probability matrix associated with a symmetric M -matrix (singular or not singular), we can erase the diagonally dominant hypothesis and the random walk associated with this model will be called *Schrödinger random walk* since any symmetric M -matrix can be interpreted as a positive semi-definite Schrödinger operator on the network.

In the two last sections, we consider fundamental parameters such as mean first passage time and Kemeny's constant and express them in terms of generalized inverses of the consider M -matrix, following the guidelines given by the works of J.J. Hunter [12–15] and some of the authors in [7] for the standard case. The first author works with generalized inverses of the *probabilistic* laplacian and the second ones with generalized inverses of the *combinatorial* laplacian.

2. Preliminaries

Our work context is a finite connected graph without loops nor multiple edges, with vertex set V (with cardinality n) and edge set E , in which each edge $\{x, y\}$ has been assigned a *conductance* $c(x, y) > 0$. We call this domain a finite network and it is denoted by the triple $\Gamma = (V, E, c)$. The conductance can be considered as a symmetric function $c: V \times V \rightarrow [0, +\infty)$ such that $c(x, x) = 0$ for any $x \in V$ and moreover, vertex x is adjacent to vertex y iff $c(x, y) > 0$. Being $\mathcal{C}(V)$ the set of real functions, for each $x \in V$, we define the *degree function* $k \in \mathcal{C}(V)$ as $k(x) = \sum_{y \in V} c(x, y)$. We call *volume of Γ* to the

value $\text{vol}(\Gamma) = \sum_{x \in V} k(x) = \sum_{x,y \in V} c(x,y)$. A positive function $\omega \in \mathcal{C}(V)$ is called *weight* if $\sum_{x \in V} \omega(x)^2 = 1$.

If we give a labeling on the vertex set V , then functions can be identified with vectors in \mathbb{R}^n , and operators can be identified with square n -matrices. For the reader's convenience, matrices will be sans serif mode and vectors will be either sans serif model or boldfaced. In particular, $\mathbf{k} = (k_1, k_2, \dots, k_n)^T$ is the degree column-vector for Γ . Given a vector \mathbf{u} , $D_{\mathbf{u}}$ will denote the diagonal matrix whose elements are given by the vector \mathbf{u} and given a matrix M , we denote by M_d the diagonal matrix whose diagonal elements are given by the diagonal of M . Hence, suppose that $V = \{x_1, x_2, \dots, x_n\}$, then we will consider $c_{ij} = c(x_i, x_j)$. Every $u \in \mathcal{C}(V)$ is identified with the vector $\mathbf{u} = (u(x_1), u(x_2), \dots, u(x_n))^T \in \mathbb{R}^n$ and the combinatorial laplacian matrix is the symmetric irreducible matrix

$$L = \begin{bmatrix} k_1 & -c_{12} & \dots & -c_{1n} \\ -c_{12} & k_2 & \dots & -c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -c_{1n} & -c_{2n} & \dots & k_n \end{bmatrix}, \tag{1}$$

where $k_i = k(x_i)$, $i = 1 \dots, n$. This matrix is diagonally dominant and, hence, it is positive semidefinite. Moreover, it is singular and 0 is a simple eigenvalue whose associated eigenvector is constant, $L\mathbf{1} = 0$, where $\mathbf{1}$ is the all ones vector. The adjacency matrix is denoted by $A_c = (c_{ij})_{i,j=1}^n$. Observe that $L = D_k - A_c$.

Given a network $\Gamma = (V, E, c)$ a standard diffusion process can be defined as a time invariant *ergodic Markov chain* with transition probability matrix $P = (p_{ij})$. Each entry $p_{ij} = \frac{c_{ij}}{k_i}$ represents the probability of transition, in one step, from vertex x_i to vertex x_j , and satisfies $P\mathbf{1} = \mathbf{1}$. It is well known that any ergodic Markov chain has a stationary distribution verifying $\pi^T P = \pi$, where $\pi_i = \frac{k_i}{\text{vol}(\Gamma)}$, see [9].

In a general setting, in addition to c_{ij} , the walker that is at vertex x_i moves to one of his neighbors x_j keeping into account the node property $\omega_j = \omega(x_j)$. For instance, it can be topological, as the degree information, or another quantity as node spreading, see [10]. In this case, the transition probability matrix is given then by

$$p_{ij} = \frac{c_{ij}\omega_j}{\sum_{\ell=1}^n c_{i\ell}\omega_{\ell}} \tag{2}$$

and hence $\pi_i = \frac{\omega_i \sum_{\ell=1}^n c_{i\ell}\omega_{\ell}}{\sum_{s,t=1}^n c_{st}\omega_t\omega_s}$ is the stationary probability at state x_i .

Some of the authors considered in [4] a new transition probability associated with a random walk that keeps the spirit of the concept of effective resistance with respect to

a non-negative value and a weight. Before introducing the definition we need to recall some potential theory concepts.

The *combinatorial laplacian* or simply the *laplacian* of the network Γ is the endomorphism of $\mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function

$$\mathcal{L}(u)(x) = \sum_{y \in V} c(x, y) (u(x) - u(y)) = k(x)u(x) - \sum_{y \in V} c(x, y) u(y), \quad x \in V.$$

Given $q \in \mathcal{C}(V)$, the *Schrödinger operator* on Γ with *potential* q is the endomorphism of $\mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function $\mathcal{L}_q(u) = \mathcal{L}(u) + qu$, where $qu \in \mathcal{C}(V)$ is defined as $(qu)(x) = q(x)u(x)$; see for instance [2,6]. It is well-known that any Schrödinger operator is self-adjoint and we are interested in those Schrödinger operators that are positive semidefinite. In [2], some of the authors answered this question by using a *Doob h -transform*, a very common technique in the framework of Dirichlet forms and Markov processes. In this context, if ω is a weight, the function $q_\omega = -\omega^{-1}\mathcal{L}(\omega)$ is called *potential determined by ω* . Then, for any $u \in \mathcal{C}(V)$ and any $x \in V$ we have the following equality

$$\mathcal{L}_q(u)(x) = \frac{1}{\omega(x)} \sum_{y \in V} c(x, y)\omega(x)\omega(y) \left(\frac{u(x)}{\omega(x)} - \frac{u(y)}{\omega(y)} \right) + (q - q_\omega)(x)u(x).$$

With this terminology the characterization of positive semi-definite Schrödinger operators is given by the following result, see [2, Prop. 3.3].

Proposition 1. *The Schrödinger operator \mathcal{L}_q is positive semi-definite iff there exist $\omega \in \Omega(V)$ and $\lambda \geq 0$ such that $q = q_\omega + \lambda$. Moreover, ω and λ are uniquely determined. In addition, \mathcal{L}_q is not positive definite iff $\lambda = 0$, in which case $\langle \mathcal{L}_{q_\omega}(v), v \rangle = 0$ iff $v = a\omega$, $a \in \mathbb{R}$. In any case, λ is the lowest eigenvalue of \mathcal{L}_q and its associated eigenfunctions are multiple of ω .*

In the sequel we only consider semidefinite positive Schrödinger operators. Therefore, we fix a value $\lambda \geq 0$, a weight $\omega \in \Omega(V)$ and their associated potential $q = q_\omega + \lambda$ and \mathcal{L}_q will be denoted by $\mathcal{L}_{\lambda,\omega}$. The matrix associated with a Schrödinger operator is $L_{\lambda,\omega} = D_{k+q} - A_c$; that is, an M -matrix.

Throughout this paper we consider as main tool the matrix

$$F_{\lambda,\omega} = L_{\lambda,\omega} - \lambda\omega\omega^T$$

that is symmetric and positive semidefinite, so $F_{\lambda,\omega}$ is also an M -matrix. Therefore 0 is a simple eigenvalue of $F_{\lambda,\omega}$ and ω is the unique unitary vector such that $F_{\lambda,\omega}\omega = 0$. Under these assumptions we shall be concerned with the so-called *Poisson equation for $F_{\lambda,\omega}$ on V* :

$$\text{Given } f \in \mathbb{R}^n \text{ find } u \in \mathbb{R}^n \text{ such that } F_{\lambda,\omega}u = f. \tag{3}$$

The general result about the resolubility of the Poisson equations is given in the following well-know result. The Poisson equation with data f has solution iff $\langle \omega, f \rangle = 0$ and moreover the solution is unique up to a multiple of ω .

We call *Generalized Inverse of $F_{\lambda,\omega}$* or *1-inverse of $F_{\lambda,\omega}$* any n -matrix assigning to any $f \in \omega^\perp$ a solution of the Poisson equation $F_{\lambda,\omega}u = f$. Therefore, due to the multiplicity of the solutions for any Poisson equation there exist infinite generalized inverses of $F_{\lambda,\omega}$ and it is well known, see for instance [1, Theorem 2.2], that a matrix G is one of them iff it satisfies the identity

$$F_{\lambda,\omega}GF_{\lambda,\omega} = F_{\lambda,\omega}. \tag{4}$$

Identity (4) implies that any generalized inverse of $F_{\lambda,\omega}$ has rank greater than or equal to the rank of $F_{\lambda,\omega}$ and hence greater than or equal to $n - 1$. Therefore any generalized inverse of $F_{\lambda,\omega}$ is either invertible or 0 is a simple eigenvalue.

The notion of generalized inverses of $F_{\lambda,\omega}$ encompasses a special type of 1-inverses that are the discrete analogue of the so-called Green matrix for $F_{\lambda,\omega}$. Specifically, we call *Green matrix* any 1-inverse, generically denoted by G such that

$$F_{\lambda,\omega}G = I - \omega\omega^T; \tag{5}$$

which is equivalent to the fact $G\omega = \alpha\omega$, $\alpha \in \mathbb{R}$. In particular, we call *orthogonal Green matrix* the unique Green matrix satisfying $F_{\lambda,\omega}^\# \omega = 0$. Observe that it coincides with the group inverse of $F_{\lambda,\omega}$ and for this reason it is denoted by $F_{\lambda,\omega}^\#$.

Therefore, $F_{\lambda,\omega}^\#$ establishes an automorphism of ω^\perp such that

$$F_{\lambda,\omega}F_{\lambda,\omega}^\# = F_{\lambda,\omega}^\#F_{\lambda,\omega} = I - \omega\omega^T \quad \text{and} \quad F_{\lambda,\omega}^\#F_{\lambda,\omega}F_{\lambda,\omega}^\# = F_{\lambda,\omega}^\#.$$

3. Schrödinger random walks

In this section we re-encounter the *Schrödinger random walks* that were introduced in [4] by some of the authors. In the mentioned paper, the authors only defined the transition probability and proved Foster’s formula. In this work, we attend to give an interpretation of these probabilities as well as to study mean first passage time and to generalize the concept of Kemeny’s constant.

The probability laws governing the evolution of the random walk are given by the *(one step) transition probability matrix with respect to λ and ω* , $P_{\lambda,\omega} \in \mathcal{M}_n(\mathbb{R})$, that is defined as

$$P_{\lambda,\omega} = D_{k_\omega}^{-1}(A_c + \lambda\omega\omega^T)D_\omega,$$

where we denote by $k_\omega = (A_c + \lambda I)\omega$, the vector whose components are $(k_i + q_i)\omega_i$.

This definition keeps the spirit of the effective resistance with respect to a parameter and a weight, introduced by the authors in [3].

Observe that for any $x_i, x_j \in V$

$$\left(P_{\lambda, \omega}\right)_{ij} = \frac{(c_{ij} + \lambda \omega_i \omega_j) \omega_j}{(k_i + q_i) \omega_i} \tag{6}$$

or equivalently

$$\left(P_{\lambda, \omega}\right)_{ij} = \frac{(c_{ij} + \lambda \omega_i \omega_j) \omega_j}{\lambda \omega_i + \sum_{\ell=1}^n c_{i\ell} \omega_\ell}. \tag{7}$$

As we can see, the main novelty in our definition is the consideration of a non-negative probability of remaining at vertex x_i given by the term

$$\left(P_{\lambda, \omega}\right)_{ii} = \frac{\lambda \omega_i^3}{\lambda \omega_i + \sum_{\ell=1}^n c_{i\ell} \omega_\ell}.$$

Moreover, for any state x_i we are considering an additional jump to any of the other states of the network x_j , which probability is given by

$$\frac{\lambda \omega_i \omega_j^2}{\lambda \omega_i + \sum_{\ell=1}^n c_{i\ell} \omega_\ell}.$$

In addition, when $\lambda = 0$ we recover the definition given in Equation (2).

If we consider $\hat{c}_{ij} = c_{ij} + \lambda \omega_i \omega_j$ and $a_{ij} = \hat{c}_{ij} \omega_i \omega_j$, then

$$\begin{aligned} \left(P_{\lambda, \omega}\right)_{ij} &= \frac{(c_{ij} + \lambda \omega_i \omega_j) \omega_j}{\lambda \omega_i + \sum_{\ell=1}^n c_{i\ell} \omega_\ell} \\ &= \frac{\hat{c}_{ij} \omega_j}{\sum_{\ell=1}^n \hat{c}_{i\ell} \omega_\ell} = \frac{\hat{c}_{ij} \omega_j \omega_i}{\sum_{\ell=1}^n \hat{c}_{i\ell} \omega_\ell \omega_i} = \frac{a_{ij}}{\sum_{\ell=1}^n a_{i\ell}}, \end{aligned}$$

see Fig. 1. So, in our model, the walker jumps to a neighbor with a probability depending on the value of the conductance c_{ij} times the factor ω_j representing the desired state property, but also we add the probability depending on $\lambda \omega_i \omega_j$. In this way, we can interpret our random walk as a random walk on a complete graph in which each edge has been assigned the conductance a_{ij} , and look at the random walk as a classical one but with non-null probability of remaining at a state.

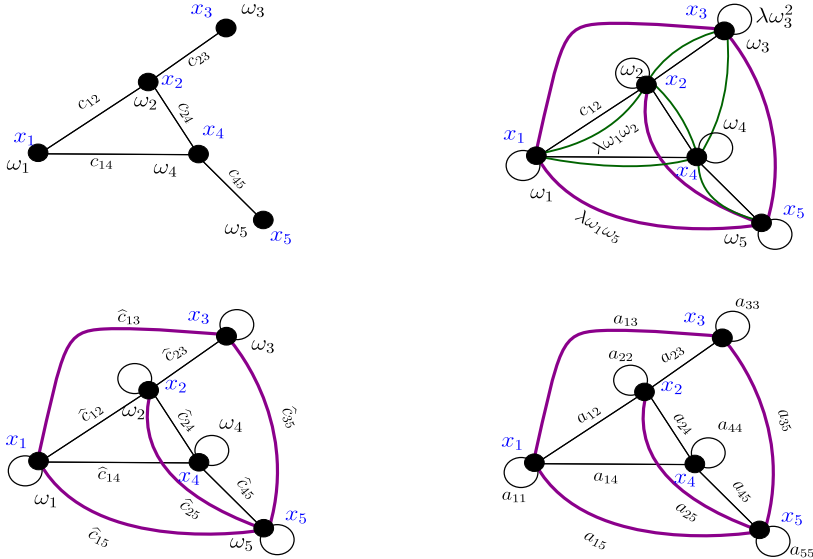


Fig. 1. Schrödinger random walks.

Consider now $\pi_{\lambda, \omega} \in \mathbb{R}^n$ defined for each $x_i \in V$ as

$$(\pi_{\lambda, \omega})_i = \frac{\lambda \omega_i^2 + \omega_i \sum_{j=1}^n c_{ij} \omega_j}{\lambda + \sum_{j, \ell=1}^n c_{j\ell} \omega_j \omega_\ell} = \frac{(k_i + q_i) \omega_i^2}{\lambda + \sum_{j, \ell=1}^n c_{j\ell} \omega_j \omega_\ell}. \tag{8}$$

We call *volume* of Γ , the value $\text{vol}(\Gamma) = \lambda + \sum_{j, \ell=1}^n c_{j\ell} \omega_j \omega_\ell$. Observe that $\text{vol}(\Gamma) = \omega^\top k_\omega$.

Lemma 1. *The transition probability matrix is markovian, reversible and has $\pi_{\lambda, \omega}$ as stationary distribution.*

Proof. It is easy to check that $\sum_{j=1}^n (P_{\lambda, \omega})_{ij} = 1$ for any $i = 1, \dots, n$, and $(\pi_{\lambda, \omega})_i (P_{\lambda, \omega})_{ij} = (\pi_{\lambda, \omega})_j (P_{\lambda, \omega})_{ji}$, for any $i, j = 1, \dots, n$. \square

In the literature we can find specific situations that can be considered as Schrödinger random walks:

- In [11], local-biased random walks on general networks where a Markovian walker is defined by different types of biases in each node to establish transitions to its neighbors depending on their degrees were considered. In this case, $\omega_j = \frac{1}{\alpha} k_j^{\beta_j}$, where $\beta = (\beta_1, \dots, \beta_n)$ is the vector defining the local bias, $\lambda = 0$ and α is the factor of normalization. Then,

$$(P_{0,\omega})_{ij} = \frac{c_{ij}k_j^{\beta_j}}{\sum_{\ell=1}^n c_{i\ell}k_\ell^{\beta_\ell}}.$$

2. In [17], the author considers core-biased random walks as a way of approximating random walks that maximize the entropy. The core-biased random walks also consider the degree sequence for defining the bias. In this case, $\omega_j = \frac{1}{\alpha} (K_j^+(k^*) + 1)$, where $K_j^+(k^*)$ is the number of links that node x_j has with nodes of degree higher or equal to k^* , $\lambda = 0$ and α is the factor of normalization. Then,

$$(P_{0,\omega})_{ij} = \frac{c_{ij}(K_j^+(k^*) + 1)}{\sum_{\ell=1}^n c_{i\ell}(K_\ell^+(k^*) + 1)}.$$

Lemma 2. For a Schrödinger random walk, it is verified that

$$D_{k_\omega} (I - P_{\lambda,\omega}) = F_{\lambda,\omega} D_\omega.$$

Proof. Observe that,

$$\begin{aligned} D_{k_\omega} (I - P_{\lambda,\omega}) &= (D_{k_\omega} - D_{k_\omega} P_{\lambda,\omega}) = (D_{k_\omega} - A_c D_\omega - \lambda \omega \omega^T D_\omega) \\ &= (D_{(k+\omega)} - A_c - \lambda \omega \omega^T) D_\omega = F_{\lambda,\omega} D_\omega. \quad \square \end{aligned}$$

In order to study mean first passage time and Kemeny’s constant for Schrödinger random walks, we are interested in obtaining the expression of any generalized inverse of the matrix $F_{\lambda,\omega}$, verifying the condition $Gk_\omega = g\omega$, in terms of its group inverse, $F_{\lambda,\omega}^\#$. Moreover, we study these expressions according to the properties verified by the generalized inverse. These results are extensions of those obtained in [15] and [7] for the case of the generalized inverses related to $I - P$ and L , respectively.

The following result was proved in [5, Theorem 3.3] in terms of operators. Here we will translate it to matrix context and we prove only the two first results that are not a direct consequence.

Theorem 1. If G is a 1-inverse of $F_{\lambda,\omega}$, then $Gk_\omega = g\omega$, $g \in \mathbb{R}$ iff there exist $\tau \in \mathbb{R}^n$ such that

$$G = F_{\lambda,\omega}^\# - \omega \tau^T - \text{vol}(\Gamma)^{-1} F_{\lambda,\omega}^\# k_\omega \omega^T,$$

and $g = -\langle \tau, k_\omega \rangle$. Moreover the following properties hold:

i) $F_{\lambda,\omega}^\# = G + \langle G\omega, \omega \rangle \omega \omega^T - \omega \omega^T G - G\omega \omega^T.$

- ii) G is invertible iff $\langle \tau, k_\omega \rangle \neq 0$ and then $G^{-1} = F_{\lambda, \omega} - \langle \tau, k_\omega \rangle^{-1} k_\omega \theta^T$, where $\theta = \omega + F_{\lambda, \omega} \tau$.
- iii) G is a symmetric matrix iff there exists $a \in \mathbb{R}$ such that

$$G = F_{\lambda, \omega}^\# + a\omega\omega^T - \frac{1}{\text{vol}(\Gamma)} \left(\omega k_\omega^T F_{\lambda, \omega}^\# + F_{\lambda, \omega}^\# k_\omega \omega^T \right);$$

that is, $\tau = \text{vol}(\Gamma)^{-1} F_{\lambda, \omega}^\# k_\omega - a\omega$. In addition, G is non singular iff $a \neq \frac{1}{\text{vol}(\Gamma)^2} \langle F_{\lambda, \omega}^\# k_\omega, k_\omega \rangle$ in which case

$$G^{-1} = F_{\lambda, \omega} + (a\text{vol}(\Gamma)^2 - \langle F_{\lambda, \omega}^\# k_\omega, k_\omega \rangle)^{-1} k_\omega k_\omega^T.$$

- iv) G is symmetric and positive semidefinite iff

$$G = F_{\lambda, \omega}^\# + a\omega\omega^T - \frac{1}{\text{vol}(\Gamma)} \left(\omega k_\omega^T F_{\lambda, \omega}^\# + F_{\lambda, \omega}^\# k_\omega \omega^T \right)$$

where $a \geq \frac{1}{\text{vol}(\Gamma)^2} \langle F_{\lambda, \omega}^\# k_\omega, k_\omega \rangle$.

- v) $G_{k_\omega} = F_{\lambda, \omega}^\# + \frac{1}{\text{vol}(\Gamma)^2} \langle F_{\lambda, \omega}^\# k_\omega, k_\omega \rangle \omega\omega^T - \frac{1}{\text{vol}(\Gamma)} \left(\omega k_\omega^T F_{\lambda, \omega}^\# + F_{\lambda, \omega}^\# k_\omega \omega^T \right)$ is the unique symmetric positive semidefinite generalized inverse that assigns to k_ω the null function.

Proof. If G is a 1-inverse of $F_{\lambda, \omega}$, from [5, Theorem 3.3], there exist $\tau, \sigma \in \mathbb{R}^n$ such that $\langle \sigma, \omega \rangle = 1$ and

$$G = F_{\lambda, \omega}^\# - \omega\tau^T - F_{\lambda, \omega}^\# \sigma\omega^T.$$

Hence, if $Gk_\omega = g\omega$, we get that

$$g\omega = Gk_\omega = F_{\lambda, \omega}^\# k_\omega - \omega\tau^T k_\omega - F_{\lambda, \omega}^\# \sigma\omega^T k_\omega = F_{\lambda, \omega}^\# k_\omega - \langle \tau, k_\omega \rangle \omega - \langle \omega, k_\omega \rangle F_{\lambda, \omega}^\# \sigma.$$

Therefore, multiplying both sides by ω^T we get that $g = -\langle \tau, k_\omega \rangle$ and $\sigma = \langle \omega, k_\omega \rangle^{-1} k_\omega = \text{vol}(\Gamma)^{-1} k_\omega$ since $\langle \sigma, \omega \rangle = 1$. Conversely, if

$$G = F_{\lambda, \omega}^\# - \omega\tau^T - \text{vol}(\Gamma)^{-1} F_{\lambda, \omega}^\# k_\omega \omega^T,$$

then, from [5, Theorem 3.3] G is a 1-inverse and $Gk_\omega = -\langle \tau, k_\omega \rangle \omega$.

To prove i), consider again the expression for $F_{\lambda, \omega}^\#$ given in [5, Theorem 3.3],

$$F_{\lambda, \omega}^\# = G - \langle \tau, \omega \rangle \omega\omega^T - \omega\omega^T G - G\omega\omega^T,$$

by imposing that $Gk_\omega = g\omega$ and keeping in mind that $\omega^T k_\omega = \text{vol}(\Gamma)$, we get that

$$F_{\lambda,\omega}^\# k_\omega = -\text{vol}(\Gamma) \left(\langle \tau, \omega \rangle \omega + G\omega \right).$$

Finally, by multiplying both sides of the above equality by ω^\top , we obtain that

$$0 = \langle F_{\lambda,\omega}^\# k_\omega, \omega \rangle = -\text{vol}(\Gamma) \left(\langle \tau, \omega \rangle + \langle G\omega, \omega \rangle \right)$$

and the result follows. \square

Corollary 1. *The symmetric and nonsingular generalized inverse of $F_{\lambda,\omega}$ such that $Zk_\omega = \omega$ is*

$$Z_{\lambda,\omega} = \left(F_{\lambda,\omega} + \frac{1}{\text{vol}(\Gamma)} k_\omega k_\omega^\top \right)^{-1}.$$

Proof. From Theorem 1 (iii), we know that if $Z_{\lambda,\omega}$ is a nonsingular and symmetric 1-inverse of $F_{\lambda,\omega}$, then there exist $a \in \mathbb{R}$ such that $\tau = \text{vol}(\Gamma)^{-1} F_{\lambda,\omega}^\# k_\omega - a\omega$. Multiplying by k_ω on both sides and keeping in mind that $g = 1$, we get that

$$-1 = \langle k_\omega, \tau \rangle = \frac{1}{\text{vol}(\Gamma)} k_\omega^\top F_{\lambda,\omega}^\# k_\omega - a \text{vol}(\Gamma).$$

Finally,

$$Z_{\lambda,\omega}^{-1} = F_{\lambda,\omega} + (\text{vol}(\Gamma))^{-1} k_\omega k_\omega^\top. \quad \square$$

From now on we will call to $Z_{\lambda,\omega}$ the *fundamental matrix with respect to λ and ω* associated with the transition probability $P_{\lambda,\omega}$. This matrix together with G_{k_ω} , the unique symmetric positive semidefinite generalized inverse that assigns to k_ω the null function, will be crucial to get simple expressions for the mean first passage time in the next section. Observe that for the standard case, these matrices are the ones obtained in [7] and moreover, $Z_{\lambda,\omega}$ is the analogue of the so-called fundamental matrix for P, Z , see [15,16].

4. Mean first passage time for Schrödinger random walks

The short-term behavior of a Schrödinger random walk is also modeled by the *mean first passage time (with respect to λ and ω)* $(m_{\lambda,\omega})_{ij}$, for $i, j = 1, \dots, n, i \neq j$, which gives the expected number of time-steps before the system reaches x_j , if it starts in x_i , then

$$(m_{\lambda,\omega})_{ij} = E[t \mid X_t = x_j, X_0 = x_i],$$

where $E[\cdot]$ denotes the expected value of the variable. It is well known [16] that, for $i \neq j, 1 \leq i, j \leq n$,

$$(m_{\lambda,\omega})_{ij} = (p_{\lambda,\omega})_{ij} + \sum_{k \neq j} (p_{\lambda,\omega})_{ik} \left((m_{\lambda,\omega})_{kj} + 1 \right) = 1 + \sum_{k \neq j} (p_{\lambda,\omega})_{ik} (m_{\lambda,\omega})_{kj}. \tag{9}$$

If we define J as the matrix of order n with all entries equal to 1, assuming that $(m_{\lambda,\omega})_{ii} = 0$ we can write (9) in matrix form as,

$$(I - P_{\lambda,\omega})M_{\lambda,\omega} = J - P(M_{\lambda,\omega})_d. \tag{10}$$

Besides, the *mean recurrence time for state x_i* , denoted by $(m_{\lambda,\omega})_{ii}$, is the expected number of time steps before we return to x_i for the first time, for any $i = 1, \dots, n$. The mean recurrence time for state x_i also verifies Equation (9) and hence its value is $\frac{1}{(\pi_{\lambda,\omega})_i}$, since multiplying both sides of (10) by $\pi_{\lambda,\omega}^T$, we obtain $\mathbf{0}^T = \pi_{\lambda,\omega}^T (J - P_{\lambda,\omega}(M_{\lambda,\omega})_d)$ or $\mathbf{0}^T = \mathbf{1}^T - \pi_{\lambda,\omega}^T (M_{\lambda,\omega})_d$.

We can use this last expression and Equation (10) to obtain the matrix expression for the MFPT.

Proposition 2. *Let Γ be a network, then the mean first passage time matrix $M_{\lambda,\omega}$, can be written as*

$$M_{\lambda,\omega} = D_{\omega}^{-1}GD_{k_{\omega}}J - JD_{\omega}^{-1}(GD_{k_{\omega}}J)_d + \text{vol}(\Gamma) \left(D_{\omega}^{-1}D_{k_{\omega}}^{-1} - D_{\omega}^{-1}GD_{\omega}^{-1} + JD_{\omega}^{-1}G_dD_{\omega}^{-1} \right).$$

In addition, for 1-inverses such that $Gk_{\omega} = g\omega$, being g a constant, we obtain

$$M_{\lambda,\omega} = \text{vol}(\Gamma) \left(D_{\omega}^{-1}D_{k_{\omega}}^{-1} - D_{\omega}^{-1}GD_{\omega}^{-1} + JD_{\omega}^{-1}G_dD_{\omega}^{-1} \right).$$

Proof. From Equation (10) and Lemma 2, we get that $(I - P_{\lambda,\omega}) = D_{k_{\omega}}^{-1}F_{\lambda,\omega}D_{\omega}$ and hence

$$\begin{aligned} F_{\lambda,\omega}D_{\omega}M_{\lambda,\omega} &= D_{k_{\omega}} \left(J - P_{\lambda,\omega}D_{\pi_{\lambda,\omega}}^{-1} \right) \\ &= D_{k_{\omega}}J - \text{vol}(\Gamma) \left(A_c + \lambda\omega\omega^T \right) D_{\omega}D_{\omega}^{-1}D_{k_{\omega}}^{-1} \\ &= D_{k_{\omega}}J - \text{vol}(\Gamma) \left(A_c + \lambda\omega\omega^T \right) D_{k_{\omega}}^{-1}. \end{aligned} \tag{11}$$

System (11) has solution because each column of the independent term belongs to ω^{\perp} and the solution is unique up to a multiple of ω , since $\langle k_{\omega}, \omega \rangle = \text{vol}(\Gamma)$ and

$$\left(\left(A_c + \lambda\omega\omega^T \right) D_{k_{\omega}}^{-1} \right)_j = \frac{1}{(k_{\omega})_j} \left((k + q)_j \varepsilon_j - (L_q)_j + \lambda\omega_j \omega_j \right)$$

and multiplying by ω^T , we get that $\frac{1}{(k_{\omega})_j} \left((k + q)_j \omega_j - \lambda\omega_j + \lambda\omega_j \right) = 1$.

Therefore, if G is a 1-inverse of $F_{\lambda,\omega}$, then

$$M_{\lambda,\omega} = D_{\omega}^{-1}G \left(D_{k_{\omega}}J - \text{vol}(\Gamma) \left(A_c + \lambda\omega\omega^T \right) D_{k_{\omega}}^{-1} \right) + JD_{\tau}.$$

By imposing the condition $(M_{\lambda,\omega})_d = \text{vol}(\Gamma)D_{\omega}^{-1}D_{k_{\omega}}^{-1}$, we get that

$$D_{\tau} = -D_{\omega}^{-1}(GD_{k_{\omega}}J)_d + \text{vol}(\Gamma)D_{\omega}^{-1} \left((G(A_c + \lambda\omega\omega^T))_d D_{k_{\omega}}^{-1} + D_{k_{\omega}}^{-1} \right).$$

Substituting in the above equation, it is verified that

$$\begin{aligned} M_{\lambda,\omega} &= D_{\omega}^{-1}GD_{k_{\omega}}J - JD_{\omega}^{-1}(GD_{k_{\omega}}J)_d \\ &\quad + \text{vol}(\Gamma)JD_{\omega}^{-1} \left((G(A_c + \lambda\omega\omega^T))_d D_{k_{\omega}}^{-1} + D_{k_{\omega}}^{-1} \right) \\ &\quad - \text{vol}(\Gamma)D_{\omega}^{-1}G \left(A_c + \lambda\omega\omega^T \right) D_{k_{\omega}}^{-1}. \end{aligned}$$

On the other hand, since G is a 1-inverse of $F_{\lambda,\omega}$, there exists $\tau \in \mathbb{R}^n$ such that

$$GF_{\lambda,\omega} = I - \omega\tau^T \implies G - G(A_c + \lambda\omega\omega^T)D_{k+q}^{-1} = D_{k+q}^{-1} - D_{\omega}JD_{\tau}D_{k+q}^{-1}$$

and hence

$$D_{\omega}^{-1}D_{k+q}^{-1} - D_{\omega}^{-1}G + D_{\omega}^{-1}G(A_c + \lambda\omega\omega^T)D_{k+q}^{-1} = JD_{\tau}D_{k+q}^{-1}.$$

If we consider the diagonal matrices associated with the matrices involved in the last equation and multiply it by J , we get that

$$JD_{\omega}^{-1}D_{k+q}^{-1} - JD_{\omega}^{-1}G_d + JD_{\omega}^{-1}(G(A_c + \lambda\omega\omega^T))_d D_{k+q}^{-1} = JD_{\tau}D_{k+q}^{-1}.$$

Therefore,

$$\begin{aligned} &JD_{\omega}^{-1}D_{k+q}^{-1} - JD_{\omega}^{-1}G_d + JD_{\omega}^{-1}(G(A_c + \lambda\omega\omega^T))_d D_{k+q}^{-1} \\ &= D_{\omega}^{-1}D_{k+q}^{-1} - D_{\omega}^{-1}G + D_{\omega}^{-1}G(A_c + \lambda\omega\omega^T)D_{k+q}^{-1} \end{aligned}$$

and hence

$$\begin{aligned} &JD_{\omega}^{-1}D_{k+q}^{-1} + JD_{\omega}^{-1}(G(A_c + \lambda\omega\omega^T))_d D_{k+q}^{-1} - D_{\omega}^{-1}G(A_c + \lambda\omega\omega^T)D_{k+q}^{-1} \\ &= D_{\omega}^{-1}D_{k+q}^{-1} - D_{\omega}^{-1}G + JD_{\omega}^{-1}G_d. \end{aligned}$$

By multiplying by D_{ω}^{-1} both sides of the above equality we get that

$$\begin{aligned} & JD_{\omega}^{-1}D_{k_{\omega}}^{-1} + JD_{\omega}^{-1}(G(A_c + \lambda\omega\omega^T))_dD_{k_{\omega}}^{-1} - D_{\omega}^{-1}G(A_c + \lambda\omega\omega^T)D_{k_{\omega}}^{-1} \\ &= D_{\omega}^{-1}D_{k_{\omega}}^{-1} - D_{\omega}^{-1}GD_{\omega}^{-1} + JD_{\omega}^{-1}G_dD_{\omega}^{-1} \end{aligned}$$

and the result follows.

Finally, if $Gk_{\omega} = g\omega$, then $D_{\omega}^{-1}GD_{k_{\omega}}J = JD_{\omega}^{-1}(GD_{k_{\omega}}J)_d = gJ$, which complete the proof. \square

5. Kemeny’s constant for Schrödinger random walks

In this section we consider the well-known parameter associated with a random walk, *Kemeny’s constant*. It represents the time for reaching a random state x_j , starting from an initial state x_i according to the stationary distribution. In our case, we define the *Kemeny’s constant (with respect to λ and ω)* as the value

$$K(M_{\lambda,\omega}) = \sum_{j=1}^n (m_{\lambda,\omega})_{ij}(\pi_{\lambda,\omega})_j.$$

In the standard case, it is a known fact that K does not depend on x_i , and hence the name *Kemeny’s constant*. In our case, this fact is also true as we will see. In a matrix-vector form, it is written as $M_{\lambda,\omega}\pi_{\lambda,\omega} = K(M_{\lambda,\omega})\mathbf{1}$.

Our aim now is to express Kemeny’s constant by using some specific 1-inverses of $F_{\lambda,\omega}$.

Proposition 3. *If G is a 1-inverse of $F_{\lambda,\omega}$ such that $Gk_{\omega} = g\omega$, Kemeny’s constant is given by*

$$K(M_{\lambda,\omega}) = 1 - g + \text{tr}(GD_{q+k}). \tag{12}$$

In particular, $K(M_{\lambda,\omega}) = \text{tr}(Z_{\lambda,\omega}D_{q+k})$ and $K(M_{\lambda,\omega}) = 1 + \text{tr}(G_{k_{\omega}}D_{q+k})$.

Proof. If we consider G a 1-inverse of $F_{\lambda,\omega}$ such that $Gk_{\omega} = g\omega$, then by Proposition 2 we get that

$$M_{\lambda,\omega}\pi_{\lambda,\omega} = \left(D_{\omega}^{-1}D_{k_{\omega}}^{-1} - D_{\omega}^{-1}GD_{\omega}^{-1} + JD_{\omega}^{-1}G_dD_{\omega}^{-1} \right) D_{\omega}k_{\omega} = [1 - g + \text{tr}(GD_{q+k})]\mathbf{1},$$

and the expression for $K(M_{\lambda,\omega})$ follows. In particular, as $Z_{\lambda,\omega}k_{\omega} = \omega$ and $G_{k_{\omega}}k_{\omega} = 0$ the last expressions for $K(M_{\lambda,\omega})$ hold. \square

Under the conditions of the above proposition, we can derive a new equation for $K(M_{\lambda,\omega})$ involving the group inverse of $F_{\lambda,\omega}$. In the case of networks and the combinatorial laplacian, a similar formula was deduced by Wang et al. in [18] using different tools and by some of the authors in [7].

Proposition 4. *In terms of the group inverse of $F_{\lambda,\omega}$, $F_{\lambda,\omega}^\#$, Kemeny’s constant is given by*

$$K(M_{\lambda,\omega}) = 1 + \text{tr}(F_{\lambda,\omega}^\# D_{k+q}) - \text{vol}(\Gamma)^{-1} k_\omega^\top F_{\lambda,\omega}^\# k_\omega. \tag{13}$$

Proof. We consider any 1-inverse of $F_{\lambda,\omega}$, such that $Gk_\omega = -\langle \tau, k_\omega \rangle \omega$, then the relation with its group inverse, given in Theorem 1, is $G = F_{\lambda,\omega}^\# - \omega \tau^\top - \text{vol}(\Gamma)^{-1} F_{\lambda,\omega}^\# k_\omega \omega^\top$. So, using Expression (12), we just have to calculate

$$\text{tr}(GD_{k+q}) = \text{tr}(F_{\lambda,\omega}^\# D_{k+q}) - \text{tr}(\omega \tau^\top D_{k+q}) - \text{vol}(\Gamma)^{-1} \text{tr}\left(F_{\lambda,\omega}^\# k_\omega \omega^\top D_{k+q}\right).$$

It is easy to see that $\text{tr}(\omega \tau^\top D_{k+q}) = \langle \tau, k_\omega \rangle$.

On the other hand, as $F_{\lambda,\omega}^\# k_\omega \omega^\top D_{k+q} = F_{\lambda,\omega}^\# k_\omega k_\omega^\top$. Then,

$$\text{tr}(F_{\lambda,\omega}^\# k_\omega \omega^\top D_{k+q}) = k_\omega^\top F_{\lambda,\omega}^\# k_\omega.$$

Hence, we get $\text{tr}(GD_{k+q}) = \text{tr}(F_{\lambda,\omega}^\# D_{k+q}) - \langle \tau, k_\omega \rangle - \text{vol}(\Gamma)^{-1} k_\omega^\top F_{\lambda,\omega}^\# k_\omega$ and finally Equation (13) holds. \square

Declaration of competing interest

The authors declare that there are no competing interests.

Data availability

No data was used for the research described in the article.

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