Kemeny's constant in Schrödinger Random Walks

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1 Introduction

We aim to generalize the transition probability matrix for a random walk on finite networks by defining the transition probabilities through a symmetric M-matrix. This new model will have special importance in applications where it is necessary to consider the possible different properties of each network node that models the random walk. We call it *Schrödinger random walk*. Unlike most models for random walks, which are based on the fact that in each step the walker moves from one node to another differently and they do not include the probability of remaining at a state, the Schrödinger random walk contemplates this possibility.

For this model, we consider the well-known parameters, mean first passage time, and Kemeny's constant, which provide a deep description of networks. As we explained, these parameters can be written using a new matrix we introduce to describe our model. We will call it *generalized Schrödinger matrix*, and it turns out to be symmetric and positive semidefinite, so it is an M-matrix.

Furthermore, we show that it is possible to express these two parameters using the so-called equilibrium measure and the equilibrium matrix, a Green matrix for the M-matrix mentioned above.

2 Schrödinger random walks

The work context is a connected network Γ. The set of vertices, also called states, is V, with $|V| = n$, and the set of edges E, with $|E| = n$. To each adjacent pair of vertices, $x \sim y$, we assign a *conductance* $c(x, y) > 0$, defined by the function $c : V \times V \longrightarrow [0, +\infty)$. The degree of vertex x is $k(x) = \sum_{y \in V} c(x, y)$, where $k \in \mathcal{C}(V)$, being $\mathcal{C}(V)$ the set of real functions on V. Finally, a *weight* is a positive function $\omega \in \mathcal{C}(V)$ such that $\sum_{x \in V} \omega(x)^2 = 1$.

Because we give an order on V, it is possible to identify operators with matrices and functions with vectors. In particular, $\mathsf{k} = \big(k_1, k_2, \ldots, k_n\big)^{\mathsf{T}}$ is the degree column-vector for Γ. $\mathsf{D_u}$ will denote the diagonal matrix whose elements are given by the vector u and given a matrix X, we denote by X_d the diagonal matrix whose diagonal elements are given by the diagonal of X. Hence, suppose that $V = \big\{x_1, x_2, \ldots, x_n\big\}$, then we will consider $c_{ij} = c(x_i, x_j)$ and we denote by A_c the adjacency

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matrix.

The combinatorial Laplacian is identified with the symmetric irreducible matrix

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

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 $\mathsf{L}\mathbf{1} = \mathbf{0}$, where $\mathbf{1}$ is the all ones vector.

A standard diffusion process in a network $\Gamma = (V, E, c)$ defines a time-invariant *ergodic Markov chain* with transition probability matrix $\mathsf{P} = (p_{ij})$, where $p_{ij} = \dfrac{c_{ij}}{k_i}$ represents the probability of transition, in one step, from vertex x_i to vertex x_j. It is well known that any ergodic Markov chain has a stationary distribution verifying $\pi^{\mathsf{T}}\mathsf{P} = \pi$, being $\pi_i = \dfrac{k_i}{\mathsf{vol}(\Gamma)}$, see [3].
In a general situation, in addition to c_{ij}, it is necessary to take into account the node property $\omega_j = \omega(x_j)$ when the walker moves to vertex x_j from x_i. In this case, the transition probability matrix is given by

$$p_{ij} = \frac{c_{ij}\omega_j}{\sum\limits_{\ell=1}^{n} c_{i\ell}\omega_\ell}, \tag{1}$$

and hence the stationary probability at state x_i is $\pi_i = \dfrac{\omega_i \sum\limits_{\ell=1}^{n} c_{i\ell\omega_\ell}}{\sum\limits_{s,t=1}^{n} c_{st}\omega_t\omega_s}$.
We are interested in positive semidefinite Schrödinger operators. So, we set $\lambda \geq 0$, a weight $\omega \in \Omega(V)$ and their associated potential defined as $q = q_\omega + \lambda$, where the potential determined by ω is defined by the vector $\big(q_\omega\big)_i = -\boldsymbol{\omega}_i^{-1}\left(\mathsf{L}\boldsymbol{\omega}\right)_i$ is . The matrix associated with $\mathsf{L}_{\lambda,\omega} = \mathsf{L} + \mathsf{D}_\mathsf{q}$ is

$$\mathsf{L}_{\lambda,\omega} = \begin{bmatrix} k_1 + q_1 & -c_{12} & \dots & -c_{1n} \\ -c_{12} & k_2 + q_2 & \dots & -c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -c_{1n} & -c_{2n} & \dots & k_n + q_n \end{bmatrix} = \mathsf{D}_{\mathsf{k+q}} - \mathsf{A}_c, \tag{2}$$

with $k_i + q_i = \lambda + \dfrac{1}{\omega_i}\sum\limits_{j=1}^{n} c_{ij}\omega_j$. This matrix is symmetric, positive semidefinite, and singular when $\lambda = 0$. Moreover, $\mathsf{L}_{\lambda,\omega}\boldsymbol{\omega} = \lambda\boldsymbol{\omega}$. When $\lambda = 0$ and $\boldsymbol{\omega}$ is constant, we recover the standard combinatorial Laplacian.

In the work, we will consider *Schrödinger random walks* that were introduced in [6] by some of the authors and studied more deeply in [3]. This model's probability depends on ω_i, ω_j and λ. Hence, and keeping in mind the case given by (1), we can write, for any $x_i, x_j \in V$,

$$p_{ij} = \frac{\big(c_{ij} + \lambda\,\omega_i\omega_j\big)\omega_j}{\big(k_i + q_i\big)\omega_i} = \frac{\big(c_{ij} + \lambda\,\omega_i\omega_j\big)\omega_j}{\lambda\omega_i + \sum\limits_{\ell=1}^{n} c_{i\ell}\omega_\ell}. \tag{3}$$

Moreover, with this model, the probability of remaining at vertex x_i is non-negative,

$$p_{ii} = \frac{\lambda\,\omega_i^2}{k_i + q_i}.$$

So, the probability laws governing the evolution of a Schrödinger random walk are given by the (*one step*) *transition probability matrix with respect to* λ *and* ω, $\mathsf{P}_{\lambda,\omega} \in M_n(\mathbb{R})$, that we can define as

$$\mathsf{P}_{\lambda,\omega} = \mathsf{D}_{\mathsf{k}_\omega}^{-1}\big(\mathsf{A}_c + \lambda\boldsymbol{\omega}\boldsymbol{\omega}^{\mathsf{T}}\big)\mathsf{D}_{\boldsymbol{\omega}},$$

where we denote by $\mathsf{k}_\omega = (\mathsf{A}_c + \lambda\mathsf{I})\boldsymbol{\omega}$, the vector whose components are $(k_i + q_i)\omega_i$.

Taking into account the previous definitions, $\boldsymbol{\pi}_{\lambda,\omega} \in \mathbb{R}^n$ can be defined for each $x_i \in V$ as

$$\big(\pi_{\lambda,\omega}\big)_i = \frac{(k_i + q_i)\omega_i^2}{\lambda + \sum\limits_{j,\ell=1}^{n} c_{j\ell}\omega_j\omega_\ell}. \tag{4}$$

We call *volume of* Γ, the value $\mathsf{vol}(\Gamma) = \lambda + \sum\limits_{j,\ell=1}^{n} c_{j\ell}\omega_j\omega_\ell$, that can be written as $\mathsf{vol}(\Gamma) = \boldsymbol{\omega}^{\mathsf{T}}\mathsf{k}_\omega$.

Lemma 1 *The transition probability matrix is reversible, Markovian, with* $\boldsymbol{\pi}_{\lambda,\omega}$ *as stationary distribution.*

The main tool for our study will be the matrix

$$\mathsf{F}_{\lambda,\omega} = \mathsf{L}_{\lambda,\omega} - \lambda\boldsymbol{\omega}\boldsymbol{\omega}^{\mathsf{T}},$$

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

$$\textit{Given } \mathsf{f} \in \mathbb{R}^n \textit{ find } \mathsf{u} \in \mathbb{R}^n \textit{ such that } \mathsf{F}_{\lambda,\omega}\mathsf{u} = \mathsf{f}. \tag{5}$$

The Poisson equation with data f has a solution iff $\langle\boldsymbol{\omega}, \mathsf{f}\rangle = 0$ and the solution is unique up to a multiple of $\boldsymbol{\omega}$.

We call *Generalized Inverse of* $\mathsf{F}_{\lambda,\omega}$ or 1-*inverse of* $\mathsf{F}_{\lambda,\omega}$ any n matrix assigning to any $\mathsf{f} \in \boldsymbol{\omega}^{\perp}$ a solution of the Poisson equation $\mathsf{F}_{\lambda,\omega}\mathsf{u} = \mathsf{f}$. So, because the solution for any Poisson equation is not unique, there are an infinite number of generalized inverses of $\mathsf{F}_{\lambda,\omega}$ and it is well known, for instance [1, Theorem 2.2], that a matrix G is one of them if and only if it satisfies the identity

$$\mathsf{F}_{\lambda,\omega}\mathsf{G}\mathsf{F}_{\lambda,\omega} = \mathsf{F}_{\lambda,\omega}, \tag{6}$$

and any generalized inverse of $\mathsf{F}_{\lambda,\omega}$ is either non singular or 0 is a simple eigenvalue.

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

$$\mathsf{F}_{\lambda,\omega}\mathsf{G} = \mathsf{I} - \boldsymbol{\omega}\boldsymbol{\omega}^{\mathsf{T}}; \tag{7}$$

which is equivalent to the fact $\mathsf{G}\boldsymbol{\omega} = \alpha\,\boldsymbol{\omega}$, $\alpha \in \mathbb{R}$. In particular, we call *Group inverse*, denoted by $\mathsf{F}_{\lambda,\omega}^{\#}$, the unique Green matrix verifying $\mathsf{F}_{\lambda,\omega}^{\#}\boldsymbol{\omega} = 0$.

The group inverse matrix is symmetric positive semidefinite. Therefore, $\mathsf{F}^{\#}_{\lambda,\omega}$ establishes an automorphism of $\boldsymbol{\omega}^{\perp}$ such that

$$\mathsf{F}_{\lambda,\omega}\mathsf{F}^{\#}_{\lambda,\omega} = \mathsf{F}^{\#}_{\lambda,\omega}\mathsf{F}_{\lambda,\omega} = \mathsf{I} - \boldsymbol{\omega}\boldsymbol{\omega}^{\mathsf{T}} \quad \text{and} \quad \mathsf{F}^{\#}_{\lambda,\omega}\mathsf{F}_{\lambda,\omega}\mathsf{F}^{\#}_{\lambda,\omega} = \mathsf{F}^{\#}_{\lambda,\omega}.$$

3 MFPT and Kemeny's constant for Schrödinger random walks

In the paper *Random Walks associated with symmetric M-matrices*, see [3], the authors focus on the study of the Kemeny's constant and, previously, the Mean first passage time, for Schrödinger random walks through the use of 1-inverses. For this, we were interested in obtaining the expression of any generalized inverse of the matrix $\mathsf{F}_{\lambda,\omega}$, verifying the condition $\mathsf{Gk}_{\omega} = g\boldsymbol{\omega}$, in terms of its group inverse, $\mathsf{F}^{\#}_{\lambda,\omega}$. Moreover, we studied these expressions according to the properties verified by the generalized inverse.

Remember that the short-term behavior of a Schrödinger random walk is modeled by the *mean first passage time* (*concerning* λ *and* ω), MFPT for now, $\big(m_{\lambda,\omega}\big)_{ij}$, for $i, j = 1, \ldots, n$, $i \neq j$; that is, if the system starts in x_i, MFPT is the expected number of time-steps before the system reaches x_j,

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

where $E[\cdot]$ denotes the expected value of the variable. We can write MFPT in a matrix form as

$$\big(\mathsf{I} - \mathsf{P}_{\lambda,\omega}\big)\mathsf{M}_{\lambda,\omega} = \mathsf{J} - \mathsf{P}(\mathsf{M}_{\lambda,\omega})_d. \tag{8}$$

Besides, the *mean recurrence time for state* x_i, $\big(m_{\lambda,\omega}\big)_{ii}$, is the expected number of time steps before we return to x_i for the first time, for any $i = 1, \ldots, n$ and its value is $\dfrac{1}{(\pi_{\lambda,\omega})_i}$.

Proposition 1 *Let* Γ *be a network, then the mean first passage time matrix* $\mathsf{M}_{\lambda,\omega}$, *can be written as*

$$\mathsf{M}_{\lambda,\omega} = \mathsf{D}^{-1}_{\boldsymbol{\omega}}\mathsf{G}\mathsf{D}_{\mathsf{k}_{\omega}}\mathsf{J} - \Big(\mathsf{D}^{-1}_{\boldsymbol{\omega}}\mathsf{G}\mathsf{D}_{\mathsf{k}_{\omega}}\mathsf{J}\Big)^{\top} + \mathsf{vol}(\Gamma)\Big(\mathsf{D}^{-1}_{\boldsymbol{\omega}}\mathsf{D}^{-1}_{\mathsf{k}_{\omega}} - \mathsf{D}^{-1}_{\boldsymbol{\omega}}\mathsf{G}\mathsf{D}^{-1}_{\boldsymbol{\omega}} + \mathsf{J}\mathsf{D}^{-1}_{\boldsymbol{\omega}}\mathsf{G}_d\mathsf{D}^{-1}_{\boldsymbol{\omega}}\Big).$$

In addition, for 1*-inverses such that* $\mathsf{Gk}_{\omega} = g\boldsymbol{\omega}$, *being* g *a constant, we obtain*

$$\mathsf{M}_{\lambda,\omega} = \mathsf{vol}(\Gamma)\Big(\mathsf{D}^{-1}_{\boldsymbol{\omega}}\mathsf{D}^{-1}_{\mathsf{k}_{\omega}} - \mathsf{D}^{-1}_{\boldsymbol{\omega}}\mathsf{G}\mathsf{D}^{-1}_{\boldsymbol{\omega}} + \mathsf{J}\mathsf{D}^{-1}_{\boldsymbol{\omega}}\mathsf{G}_d\mathsf{D}^{-1}_{\boldsymbol{\omega}}\Big).$$

Now, we will 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 *Kemeny's constant (with respect to* λ *and* ω*)* as the value

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

In the standard case, it is known that K does not depend on x_i, hence the name *Kemeny's constant*. In a matrix-vector form, it is written as $\mathsf{M}_{\lambda,\omega}\boldsymbol{\pi}_{\lambda,\omega} = K(\mathsf{M}_{\lambda,\omega})\mathsf{1}$.

Under the conditions of the next proposition, we can derive a new equation for $K(\mathsf{M}_{\lambda,\omega})$ involving the group inverse of $\mathsf{F}_{\lambda,\omega}$.

Proposition 2 *If* G *is a* 1*-inverse of* $\mathsf{F}_{\lambda,\omega}$ *such that* $\mathsf{Gk}_\omega = g\boldsymbol{\omega}$*, Kemeny's constant is given by*

$$K(\mathsf{M}_{\lambda,\omega}) = 1 - g + \mathrm{tr}(\mathsf{GD}_{\mathsf{q+k}}). \tag{9}$$

Indeed, we have the proposition below.

Proposition 3 *In terms of the group inverse of* $\mathsf{F}_{\lambda,\omega}$*,* $\mathsf{F}^{\#}_{\lambda,\omega}$*, Kemeny's constant is given by*

$$K(\mathsf{M}_{\lambda,\omega}) = 1 + \mathsf{tr}(\mathsf{F}^{\#}_{\lambda,\omega}\mathsf{D}_{\mathsf{k+q}}) - \mathsf{vol}(\Gamma)^{-1}\mathsf{k}_\omega{}^{\mathsf{T}}\mathsf{F}^{\#}_{\lambda,\omega}\mathsf{k}_\omega. \tag{10}$$

4 Equilibrium Measure for Schrödinger random walks

In addition to this description of Kemeny's constant in terms of any 1-inverses, we will express it using a specific Green matrix for $\mathsf{F}_{\lambda,\omega}$. This new matrix will be defined from the concept of *equilibrium measure*.

So, given a vertex subset $F \subset V$, it can be considered a function $\nu^F_{\lambda,\omega} \in \mathcal{C}(F)$ such that $\mathcal{L}_{\lambda,\omega}(\nu^F_{\lambda,\omega}) = \omega$. We will call that function *equilibrium measure of* F *concerning* λ *and* ω. Moreover, $\nu^F_{\lambda,\omega}$ is unique and $\nu^F_{\lambda,\omega} > 0$, on F. Additionally, the value $\mathsf{cap}_{\lambda,\omega}(F) = \langle \omega, \nu^F_{\lambda,\omega}\rangle$ is called *capacity of* F. The equilibrium measure and the capacity of the set $V \setminus \{x_i\}$ are denoted by $\nu^i_{\lambda,\omega}$ and by $\mathsf{cap}_{\lambda,\omega}(x_i)$.

From the definition of $\nu^i_{\lambda,\omega}$ and $\mathsf{cap}_{\lambda,\omega}(x_i)$, we will consider what we will call *equilibrium matrix with respect to* λ *and* ω, $\mathsf{E}_{\lambda,\omega}$, which can be demonstrate is a Green matrix for $\mathsf{F}_{\lambda,\omega}$. Then, we will obtain explicit expressions for MFPT regarding the equilibrium measure and Kemeny's constant with respect to the equilibrium matrix.

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