Group Inverse and equilibrium measure on Random Walks

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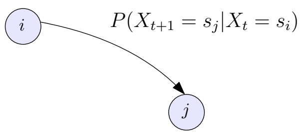
Abstract

In this manuscript we show the central role of the group inverse of the Laplacian in the study of random walks on networks. Moreover, we take advantage of the relation of group inverse and equilibrium measures and we obtain expressions for the mean first passage time and for Kemeny's constant in terms of equilibrium measures. For networks with symmetries we can obtain the analytic expression of the above parameters such as distance bi-regular graphs or barbell networks.

Our work context is a **connected network** Γ, that is, from any vertex we can reach any other one. The set of vertices, or states, is V, with $|V| = n$, and the set of edges E, with $|E| = n$. The conductance function assigns a weight to each edge. Because we give an order on the vertex set, V, it is possible identify operators with matrices and functions with vectors.

Given an initial state s_0, we move randomly to a neighbor state, s_1, and then to s_2, and so on. That process generate a sequence of states $\{s_1, s_2, \ldots, s_t, \ldots\}$ called **random walk** on Γ. In each step t we define a random variable X_t that takes values on V. That sequence of random variables defines a **discret stochastic process time**, and the probability associated with the movement from an initial state s_i to another neighbor state s_j is given by $\mathbb{P}\big(X_{t+1} = s_j | X_t = s_i\big) = \dfrac{c_{ij}}{k_i}$,



where k_i is the degree of the state s_i. This probability does not depend of the previous states,

$$\mathbb{P}\big(X_{t+1} = j | X_t = i, X_{t-1} = i_{t-1}, \ldots, X_0 = i_0\big) = \mathbb{P}\big(X_{t+1} = j | X_t = i\big),$$

so the Markov property holds and the network is memoryless. The matrix with entrances p_{ij} is called *transition probability matrix*, which is a stochastic matrix. As $\mathsf{P} \geq 0$ and irreducible (connected network), exist a left eigenvector associated with the dominant eigenvalue $\lambda = 1$ of P,

$$\boldsymbol{\pi}^{\mathrm{T}} \mathsf{P} = \boldsymbol{\pi}^{\mathrm{T}}$$

This vector $\boldsymbol{\pi}$ is unique, and its components are all positive. We can normalize the vector, so $\sum_{i=1}^{n} \pi_i = 1$, and then $\boldsymbol{\pi}$ is a probability distribution vector. In fact, $\boldsymbol{\pi}$ represents a **stationary distribution**: if, at $t = 0$, the system is in the state j with probability π_j, the probability of being in j for $t > 0$ is π_j as well.

For our convenience, we can define Π as the matrix such that all its rows are equal to vector $\boldsymbol{\pi}$, $\Pi = \mathbf{1}\boldsymbol{\pi}^{\mathsf{T}}$. This matrix allows to study the long-term behavior of the RW.

An important operator –matrix– for our work on RW is the **combinatorial Laplacian**, defined as

$$\mathsf{L} = \mathsf{D}_k - \mathsf{A},$$

where D_k is the diagonal degree matrix and $\mathsf{A} = \left(c_{ij}\right)_{i,j=1}^{n}$ the adjacency matrix, with $\mathsf{A} = \mathsf{D}_k\mathsf{P}$. L is a symmetric Z-matrix and diagonally dominant, positive semidefinite, singular and 0 is a simple eigenvalue whose associated eigenvectors are constants, $\mathsf{L}\mathbf{1} = \mathbf{0}$. The properties of L are transferred to its group inverse, $\mathsf{L}^{\#}$, which is the unique matrix such that satisfies the equations $\mathsf{L} \cdot \mathsf{L}^{\#} \cdot \mathsf{L} = \mathsf{L}$, $\mathsf{L}^{\#} \cdot \mathsf{L} \cdot \mathsf{L}^{\#} = \mathsf{L}^{\#}$, $\mathsf{L} \cdot \mathsf{L}^{\#} = \mathsf{L}^{\#} \cdot \mathsf{L}$. So $\mathsf{L}^{\#}$ it is a symmetric and diagonally dominant, positive semidefinite, and singular, with $\mathsf{L}^{\#}\mathbf{1} = \mathbf{0}$ as well. Moreover, group inverse can be characterized as follows

$$\mathsf{L}\,\mathsf{L}^{\#} = \mathsf{I} - \frac{1}{n}\mathsf{J},$$

where J is the n-matrix with all its entries equal to 1. Sot it is clear than $\mathsf{L}^{\#}$ is a 1-inverse.

Before introducing the Equilibrium measure, we state the **Minimum Principle** as follows: if $\mathsf{u} \in^n$ satisfies $\mathsf{u}_i \geq 0$ and $(\mathsf{Lu})_j \geq 0$, for any $j \neq i$, then $\mathsf{u}_j \geq 0$, for all $j = 1, \ldots, n$. Hence, it can be deduced that for each $j \in V$ there exists ν^j such that $\nu^j_j = 0$ and $\nu^j_i > 0$ for any $i \neq j$. ν^j-function is called **Equilibrium measure** of $V \setminus \{j\}$ and because we impose

$$\mathsf{L}(\nu^j_i) = \mathbf{1}, \quad \text{for all } i \neq j,$$

this function can be seen as the measure that gives equal potential in each state of $V \setminus \{j\}$. It can be proof, that the equilibrium measure of V holds

$$\mathsf{L}(\nu^j_i) = \mathbf{1} - n\mathbf{1}_j,$$

if we consider column j, and being $\mathbf{1}_j$ the j-th unit vector. By defining the so-called **equilibrium matrix** for Γ, $\mathsf{E}_{ij} = -\frac{1}{n}\nu^j_i$, $j = 1, \ldots, n$, we have

$$\mathsf{LE} = \mathsf{I} - \frac{1}{n}\mathsf{J}.$$

So, E can be seen as a 1-inverse of L.

It is possible to express the group inverse $\mathsf{L}^\#$ in terms of equilibrium measures.

The short-term behavior of the RW can be described by the **mean first passage time** (MFPT), denoted by m_{ij}; that is, the expected number of steps to reach state j for the first time if we start at state i. Its expression is very well known,

$$m_{ij} = p_{ij} + \sum_{k\neq j} p_{ik}\big(m_{kj}+1\big) = 1 + \sum_{k\neq j} p_{ik} m_{kj}.$$

In a matrix form, we can write expression for mean first passage time as $(\mathsf{I}-\mathsf{P})\mathsf{M} = \mathsf{J} - \mathsf{P}\mathsf{D}_\pi^{-1}$. Although $\Delta = \mathsf{I}-\mathsf{P}$ is a singular matrix, because of $\mathsf{J}-\mathsf{P}\mathsf{D}_\pi^{-1} \perp \ker\big(\mathsf{I}-\mathsf{P}\big)^{\mathrm{T}}$, the system is compatible since $\mathsf{J}-\mathsf{P}\mathsf{D}_\pi^{-1} \perp \ker\big(\mathsf{I}-\mathsf{P}\big)^{\mathrm{T}}$, and any 1-inverse $\widetilde{\mathsf{G}}$ of the $\mathsf{I}-\mathsf{P}$ solve the system. So,

$$\mathsf{M} = \widetilde{\mathsf{G}}\big(\mathsf{J} - \mathsf{P}\mathsf{D}_{\boldsymbol{\pi}}^{-1}\big) + \mathbf{1}\mathsf{v}^{\mathsf{T}}$$

is its general solution.

We can express the 1-inverse for the combinatorial Laplacian, $\widetilde{\mathsf{G}}$, in terms of the 1-inverse of the probabilistic Laplacian, G, $\mathsf{G} = \widetilde{\mathsf{G}}\mathsf{D}_k^{-1}$. So, if G is any 1-inverse of L, then:

$$\mathsf{M} = \mathsf{G}\mathsf{D}_k\mathsf{J} - \mathsf{J}\big(\mathsf{G}\mathsf{D}_k\mathsf{J}\big)_d + \mathrm{vol}(\Gamma)\Big(\mathsf{D}_k^{-1} - \mathsf{G} + \mathsf{J}\mathsf{G}_d\Big).$$

Of all possible 1-inverses, we choose those such that fulfill the property $\mathsf{G}\mathsf{k} = g\mathbf{1}$, and in that case

$$\mathsf{M} = \mathrm{vol}(\Gamma)\Big(\mathsf{D}_k^{-1} - \mathsf{G} + \mathsf{J}\mathsf{G}_d\Big).$$

On the other hand, our research group has established the relationship between the group inverse of L, and any other 1-inverse G:

$$\mathsf{G} = \mathsf{L}^\# - \mathbf{1}\boldsymbol{\tau}^{\mathsf{T}} - \mathsf{L}^\#\boldsymbol{\pi}\mathbf{1}^{\mathsf{T}},$$

with $g = -\mathrm{vol}(\Gamma)\langle\boldsymbol{\tau},\boldsymbol{\pi}\rangle$. Moreover, there is another one symmetric positive semidefinite 1-inverse such that zero is an eigenvalue with stationary distribution as an associated eigenvector, $\mathsf{G}\boldsymbol{\pi} = \mathbf{0}$,

$$\mathsf{G}_{\boldsymbol{\pi}} = \mathsf{L}^\# + \boldsymbol{\pi}^{\mathsf{T}}\mathsf{L}^\#\boldsymbol{\pi}\mathsf{J} - \Pi\mathsf{L}^\# - \mathsf{L}^\#\Pi^{\mathsf{T}}.$$

So,

$$\mathsf{M} = \mathrm{vol}(\Gamma)\Big(\mathsf{D}_{\mathsf{k}}^{-1} - \mathsf{L}^\# + \mathsf{J}\mathsf{L}_d^\# + \Pi\mathsf{L}^\# + \mathsf{L}^\#\Pi^{\mathsf{T}} - 2\mathsf{J}\mathsf{D}_{\mathsf{L}^\#\boldsymbol{\pi}}\Big).$$

Moreover, it can be written a relation between the equilibrium measure and the MFPT.

On the other side, Kemeny's constant is a parameter that measures the time for reaching a random state s_j, starting from an initial one s_i, according to the stationary distribution. It is remarkable that K is independent of the starting state, s_i.

It is customary to take as the definition of the Kemeny's constant the following:

$$K = \sum_{j \in V} m_{ij} \pi_j.$$

Some authors take as definition of Kemenys constant $K' = 1 - K$. In that case, it is taken $t \geq 0$ in the definition of MFPT.

As we are interested in the combinatorial Laplacian, and its group inverse, we have obtained the Kemeny's constant in terms of $\mathsf{L}^{\#}$:

$$K = 1 + \mathbf{1}^{\mathsf{T}} \mathsf{L}_d^{\#} \mathsf{k} - \frac{1}{\mathrm{vol}(\Gamma)} \mathsf{k}^{\mathsf{T}} \mathsf{L}^{\#} \mathsf{k}.$$

And, again, it is possible to write Kemeny's constant in terms of the new function defined before, equilibrium measures of $V \setminus \{j\}$, $j = 1, \ldots, n$.

Finally, the case of the Wheel network will be introduced, as an example of the power of the use of group inverse of L and the equilibrium measures to calculate MFPT and Kemeny's constant, specially when the network is not simle enough.

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