g-inverses for Random Walks

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In terms of random walks skills, if we asume that the system is in an initial state s_i, the number of expected steps to reach state s_j is described by the so-called Mean First Passage Time (MFPT), which is denoted by m_{ij}. The matrix characterizing the MFPT can be written in terms of the g-inverses of the combinatorial Laplacian, see [1].

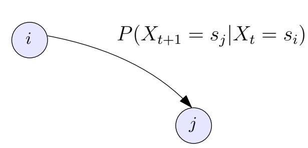
Although the MFPT is an element that allows to describe random walks, it is not the only one. It is well known that the time to reach a random state s_j, starting from an initial state s_i, is a constant that does not depend of the initial state. This time is the so-called Kemeny's constant, that it can be expressed in terms of g-inverses of the above-mentioned Laplacian.

We will obtain expressions both for the MFPT and for the Kemeny's constant in terms of g-inverses of the combinatorial Laplacian. In addition, as an application, we introduce the case of the star.

In this talk, we want to explain how we can use g-inverses as resolvents to calculate some elements that allow us to characterize simple random walks: the Mean First Passage Time and the Kemeny's constant.

We will start with some basic definitions. Let Γ a *connected network*, that is, from any vertex we can reach any other one. The set of vertices will be V (there are n vertices) and the set of edges E (there are m edges). The conductance function assigns a weight to each edge. In fact, according to the nomenclature used in stochastic processes, it is preferible to talk, not about vertices, but states.

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 *simple 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. What does *random* mean? Let's supose we are in a state s_i at a time t. Then there's a probability $P\big(X_{t+1} = s_j | X_t = s_i\big)$ associated with the movement to another neighbor state s_j.



Being k_i the grade of state s_i, the sum of conductances, then this probability will be $\frac{c_{ij}}{k_i}$. Observe that, in general, the probability $i \to j$ is not the same that the probability of $j \to i$. The probability $P\big(X_{t+1} = j | X_t = i\big)$ does not depend of the previous states,

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

and we say that the random walk holds the Markov property. The matrix with entrances p_{ij} is called *transition probability matrix*, which is a stochastic matrix. Entry ij-th of P^t matrix represents the probability of reaching state j after t steps if the system starts at state i. Being u_0 the initial distribution vector, $\mathsf{u}_t^{\mathsf{T}} = \mathsf{u}_0^{\mathsf{T}} \mathsf{P}^t$, is the probability distribution after t steps.

As $\mathsf{P} \geq 0$ and irreducible (connected network), the Perron-Frobenius theorem guarantees the existence of a left eigenvector associated with the dominant eigenvalue $\lambda = 1$ of P,

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

This vector $\boldsymbol{\pi}$ is unique, and any other eigenvalue of P is $\mu \leq \lambda = 1$. The components of $\boldsymbol{\pi}$ are all positive and we can normalize the vector, so $\displaystyle\sum_{i=1}^{n} \pi_i = 1$. 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.

Let's consider the long-term behavior of the RW. We define Π as the matrix such that all its rows are equal to vector $\boldsymbol{\pi}$. Then, for regular random walks,

$$\Pi = \lim_{t \to +\infty} P^t;$$

that is, the probability of reaching any state j is independent of the initial state and it is equal to π_j.

After that, we want to introduce to important matrices in random walks: $\mathsf{I} - \mathsf{P}$, the *probabilistic Laplacian* of the network, and the *combinatorial Laplacian*, with which our research group prefers to work:

$$\mathsf{L} = \mathsf{D}_k - \mathsf{A} = \mathsf{D}_k \cdot (\mathsf{I} - \mathsf{P}).$$

Both probabilistic Laplacian and combinatorial are singular matrices, so they have 0 as a less eigenvalue, hence they have constants as proper functions. Moreover, the stationary distribution is an eigenvector of the transpose matrix of the probabilistic Laplacian:

$$\boldsymbol{\pi}^{\mathrm{T}} \big(\mathsf{I} - \mathsf{P}\big) = \mathbf{0} \Leftrightarrow \big(\mathsf{I} - \mathsf{P}\big)^{\mathrm{T}} \boldsymbol{\pi} = \mathbf{0}$$

That means that de stationary distribution belongs to the ker of the matrix $\big(\mathsf{I} - \mathsf{P}\big)^{\mathrm{T}}$.

Agfter the long-term behavior of the RW, we analyze the short-term one. Suppose that we are at state i. The expected number of steps to reach state j for the first time is called *mean first passage time*, denoted by m_{ij}.

If we consider $i \neq j$, once we have taken de first step, we mesure the number of steps to get final state j and then multiple by the associated probability in each step. If the first step is to j, the number of steps is 1. If to another state k, the required number of steps is m_{kj} plus 1, because the previous step done, $i \to k$. So,

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

If cas $i = j$, m_{ii} is the expected number of steps to return to state i. It is called de *mean recurrence time* for i and can be calculated as $m_{ii} = \dfrac{1}{\pi_i}$.

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

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

Hunter (1982) gave the solution in terms of any 1-inverse

$$\mathsf{M} = \Big[\mathsf{G}\Pi - \mathsf{J}\big(\mathsf{G}\Pi\big)_d + \mathsf{I} - \mathsf{G} + \mathsf{J}\mathsf{G}_d\Big]\mathsf{D}_\pi^{-1}.$$

Hunter himself showed (2008) that the previous expression can be simplified if we consider 1-inverses of the form $\mathsf{G}\mathbf{1} = g\mathbf{1}$, being g a constant. That's equivalent to the condition $\mathsf{G}\Pi - \mathsf{J}\big(\mathsf{G}\Pi\big)_d = 0$. So $\mathsf{M} = \big(\mathsf{I} - \mathsf{G} + \mathsf{J}\mathsf{G}_d\big)\mathsf{D}_\pi^{-1}$.

In 1960, Kemeny and Snell have given a solution for the matrix equation in terms of the so-called *fundamental matrix*, $\mathsf{Z} = \big(\mathsf{I} - \mathsf{P} + \Pi\big)^{-1}$. This matrix is a invertible 1-inverse, with $\mathsf{Z}\mathbf{1} = \mathbf{1}$ –that is, of the type $\mathsf{G}\mathbf{1} = g\mathbf{1}$, with $g = 1$. Efectivament, sabem que $\mathsf{P}\mathbf{1} = \mathbf{1}$ i que $\Pi\mathbf{1} = \mathbf{1} \cdot \boldsymbol{\pi}^{\mathrm{T}}\mathbf{1} = \mathbf{1} \cdot 1 = \mathbf{1}$. Aleshores,

$$\big(\mathsf{I} - \mathsf{P} + \Pi\big)\mathbf{1} = \mathbf{1} \quad \Rightarrow \quad \mathsf{Z}^{-1}\mathbf{1} = \mathbf{1} \quad \Rightarrow \quad \mathsf{Z}\mathbf{1} = \mathbf{1}$$

It can be observed that $\boldsymbol{\pi}^{\mathrm{T}}\big(\mathsf{I} - \mathsf{P} + \Pi\big) = \boldsymbol{\pi}^{\mathrm{T}}$, and so on $\boldsymbol{\pi}^{\mathrm{T}}\big(\mathsf{I} - \mathsf{P} + \Pi\big)^{-1} = \boldsymbol{\pi}^{\mathrm{T}}$. Hence $\mathsf{I} - \mathsf{Z} = \Pi - \mathsf{P}\mathsf{Z}$.
Finally, the solution for the MFPT is:

$$\mathsf{M} = \Big(\mathsf{I} - \mathsf{Z} + \mathsf{J}\mathsf{Z}_d\Big)\mathsf{D}_\pi^{-1}$$

Meyer (1975) solved the equation for M with the inverse group of the matrix $\mathsf{I}-\mathsf{P}$, given by $\big(\mathsf{I}-\mathsf{P}\big)^{\#}=\big(\mathsf{I}-\mathsf{P}+\Pi\big)^{-1}-\Pi=\mathsf{Z}-\Pi$. This matrix has 0 as a eigenvalue associated with to $\mathbf{1}$; so, is of the form $\mathsf{G}\mathbf{1}=g\mathbf{1}$ as well, with $g=0$. Indeed,

$$\big(\mathsf{I}-\mathsf{P}\big)^{\#}\mathbf{1}=\mathsf{Z}\mathbf{1}-\Pi\mathbf{1}=\mathbf{1}-\mathbf{1}=0\mathbf{1}$$

From the previous equality $\boldsymbol{\pi}^{\mathrm{T}}\big(\mathsf{I}-\mathsf{P}+\Pi\big)^{-1}=\boldsymbol{\pi}^{\mathrm{T}}$, we get $\boldsymbol{\pi}^{\mathrm{T}}\big(\mathsf{I}-\mathsf{P}\big)^{\#}=0$.

We want to note that it is possible to express the 1-inverse for the combinatorial Laplacian, $\widetilde{\mathsf{G}}$, in terms of the 1-inverse of the probabilistic Laplacian, G, as follows $\widetilde{\mathsf{G}}=\mathsf{G}\mathsf{D}_k^{-1}$. So, if G is any 1-inverse of L, then:

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

Moreover, if $\widetilde{\mathsf{G}}$ is such that $\mathsf{G}\mathbf{1}=g\mathbf{1}$, then G holds $\mathsf{G}\mathsf{k}=g\mathbf{1}$, and it that case $\mathsf{M}=\mathrm{vol}(\Gamma)\Big(\mathsf{D}_k^{-1}-\mathsf{G}+\mathsf{J}\mathsf{G}_d\Big)$.

References

[1] Á. Carmona, M.J. Jiménez, À. Martín. Generalized inverses of the combinatorial Laplacian for mean first passage times and Kemeny's constant. *Submitted*, (2022).