A GRAPH THEORETIC INTERPRETATION OF
THE MEAN FIRST PASSAGE TIMES

Pavel Chebotarev*
Institute of Control Sciences of the Russian Academy of Sciences
65 Profsoyuznaya Street, Moscow 117997, Russia

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Abstract

Let $m_{ij}$ be the mean first passage time from state $i$ to state $j$ in an $n$-state ergodic homogeneous Markov chain with transition matrix $T$. Let $G$ be the weighted digraph without loops whose vertex set coincides with the set of states of the Markov chain and arc weights are equal to the corresponding transition probabilities. We show that

$$m_{ij} = \begin{cases} 
\frac{f_{ij}}{q_j}, & \text{if } i \neq j, \\
\frac{1}{q_j}, & \text{if } i = j,
\end{cases}$$

where $f_{ij}$ is the total weight of 2-tree spanning converging forests in $G$ that have one tree containing $i$ and the other tree converging to $j$, $q_j$ is the total weight of spanning trees converging to $j$ in $G$, and $\tilde{q}_j = q_j / \sum_{k=1}^{n} q_k$. The result is illustrated by an example.

Keywords: Markov chain; Mean first passage time; Spanning rooted forest; Matrix forest theorem; Laplacian matrix

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1 Introduction

Let $T = (t_{ij}) \in \mathbb{R}^{n \times n}$ be the transition matrix of an $n$-state ergodic homogeneous Markov chain with states $1, \ldots, n$. Then $T$ is an irreducible stochastic matrix. The mean first passage time from state $i$ to state $j$ is defined as follows:

$$m_{ij} = \mathbb{E}(F_{ij}) = \sum_{k=1}^{\infty} k \Pr(F_{ij} = k),$$

*E-mail: pavel4e@gmail.com
where
\[ F_{ij} = \min\{p \geq 1 : X_p = j \mid X_0 = i\} \]  \hspace{1cm} (2)

By [6, Theorem 3.3] the matrix \( M = (m_{ij})_{n \times n} \) has the following representation:
\[ M = (I - L^\# + JL^\#_{dg})\Pi^{-1}, \]  \hspace{1cm} (3)

where \( L^\# \) is the group inverse of \( L \),
\[ L = I - T, \]  \hspace{1cm} (4)

\( J \) is the all ones matrix, \( L^\#_{dg} \) is the diagonal matrix obtained by setting all off-diagonal entries of \( L^\# \) to zero, \( \Pi = \text{diag}(\pi_1, \ldots, \pi_n) \), and \( (\pi_1, \ldots, \pi_n) = \pi \) is the normalized left Perron vector of \( T \), i.e., the row vector in \( \mathbb{R}^n \) satisfying
\[ \pi T = \pi \quad \text{and} \quad \|\pi\|_1 = 1. \]  \hspace{1cm} (5)

In an entrywise form, (3) reads as follows (see, e.g., [1]):
\[ m_{ij} = \begin{cases} 
\pi_j^{-1}, & \text{if } i = j, \\
\pi_j^{-1}(L^\#_{jj} - L^\#_{ij}), & \text{if } i \neq j. 
\end{cases} \]  \hspace{1cm} (6)

In the following section, we use this formula to derive a graph-theoretic interpretation of the mean first passage times.

2 A forest expression for the mean first passage times

Let us say that a weighted digraph \( G \) corresponds to the Markov chain with transition matrix \( T \) if the Laplacian matrix \( L \) of \( G \) satisfies (4). Let the vertex set of \( G \) be \( \{1, 2, \ldots, n\} \). Then, by (4), arc \((i, j)\) belongs to the arc set of \( G \) whenever \([i \neq j \text{ and } t_{ij} \neq 0]\); the weight of this arc is \( t_{ij} \).

Let us recall some graph-theoretic notation. A digraph is weakly connected if the corresponding undirected graph is connected. A weak component of a digraph \( G \) is any maximal weakly connected subdigraph of \( G \). An in-forest of \( G \) is a spanning subgraph of \( G \) all of whose weak components are converging trees (also called in-arborescences). A converging tree is a weakly connected digraph in which one vertex, called the root, has outdegree zero and the remaining vertices have outdegree one. An in-forest is said to converge to the roots of its converging trees. An in-forest \( F \) of a digraph \( G \) is called a maximum in-forest of \( G \) if \( G \) has no in-forest with a greater number of arcs than in \( F \). The in-forest dimension of a digraph \( G \) is the number of weak components in any maximum in-forest. Obviously, every maximum in-forest of \( G \) has \( n - d \) arcs, where \( d \) is the in-forest dimension of \( G \). A submaximum in-forest of \( G \) is an in-forest of \( G \) that has \( d + 1 \) weak components; as a consequence, it has \( n - d - 1 \) arcs.

The weight of a weighted digraph is the product of its arc weights; the weight of any digraph that has no arcs is 1. The weight of a set of digraphs is the sum of the weights of its members.
By (iii) of Proposition 15, for any weighted digraph $G$ and its Laplacian matrix $L$,
\[ L^\# = \sigma^{-1}_{n-d} \left( Q_{n-d-1} - \frac{\sigma^{-1}_{n-d-1}}{\sigma_{n-d}} Q_{n-d} \right), \]  
(7)
where $\sigma_k$ is the total weight of in-forests with $k$ arcs (so that $\sigma_{n-d}$ and $\sigma_{n-d-1}$ are the total weights of maximum and submaximum forests of $G$, respectively), $Q_k$ is the matrix whose $(i,j)$ entry ($i, j = 1, \ldots, n$) is the total weight of in-forests that have $k$ arcs and vertex $i$ belonging to the tree that converges to vertex $j$.

To obtain a forest representation of the mean first passage times, it suffices to combine (6) and (7). First, observe that since the Markov chain under consideration is ergodic, the corresponding digraph $G$ has spanning converging trees. Thus, the in-forest dimension of $G$ is 1. Consequently, for every $i, j = 1, \ldots, n$, each maximum in-forest converging to $j$ is a spanning converging tree, which contains $i$. Therefore, the $(j,j)$ and $(i,j)$ entries of $Q_{n-d} = Q_{n-d-1}$ are the same.

As a result, substituting (7) in (6) provides the differences of the form
\[ q_{jj}^{(n-2)} - q_{ij}^{(n-2)} \overset{\text{def}}{=} f_{ij} \]
(8)
between the $(j,j)$ and $(i,j)$ entries of the matrix $= (q_{ij}^{(n-2)}) = Q_{n-2} = Q_{n-d-1}$. By definition of $Q_{n-2}$, this difference equals the weight of the set of 2-tree in-forests of $G$ that converge to $j$ and have $i$ and $j$ in different trees. Thus, substituting (7) in (6) yields
\[ m_{ij} = f_{ij}/(\sigma_{n-1} \pi_j) \text{ if } i \neq j. \]
(9)

Furthermore, we know (for example, from the Markov chain tree theorem [4, 5] first obtained in [7]; see also [8, 3]) that
\[ \pi_j = q_j/\sigma_{n-1}, \]
(10)
where $q_j$ is the total weight of trees converging to $j$ in $G$, so that $\sum_{k=1}^n q_k = \sigma_{n-1}$. Eqs. (9), (10) and (6) finally provide $m_{ij} = f_{ij}/q_j$ for $i \neq j$ and $m_{jj} = (q_j/\sigma_{n-1})^{-1}$. We have proved the following theorem.

**Theorem 1** Let $T \in \mathbb{R}^{n \times n}$ be the transition matrix of an $n$-state ergodic homogeneous Markov chain with states $1, \ldots, n$. Let $G$ be the weighted digraph without loops whose vertices are $1, \ldots, n$ and arc weights are equal to the corresponding transition probabilities in $T$. Then the mean first passage times from state $i$ to state $j$ in the Markov chain can be represented as follows:
\[ m_{ij} = \begin{cases} f_{ij}/q_j, & \text{if } i \neq j, \\ 1/\tilde{q}_j, & \text{if } i = j. \end{cases} \]
(11)
where $f_{ij}$ is the total weight of 2-tree in-forests of $G$ that have one tree containing $i$ and the other tree converging to $j$, $q_j$ is the total weight of spanning trees converging to $j$ in $G$, and $\tilde{q}_j = q_j/\sum_{k=1}^n q_k$. 

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Remark 1. If one removes the subsidiary requirement $p \geq 1$ from the definition of mean first passage time (Eq. (2)), then one has $m_{jj} = 0$ and $m_{ij} = f_{ij}/q_j, \ i, j = 1, \ldots , n$, since $f_{jj} = 0$ for every $j$.

Remark 2. $f_{ij}$ and $q_j$ can be calculated by means of elementary matrix algebra, namely, by the following recurrence procedure [2, Proposition 4]. For $k = 0, 1, \ldots$, one has

$$\sigma_{k+1} = \frac{\text{tr}(LQ_k)}{k+1},$$

$$Q_{k+1} = -LQ_k + \sigma_{k+1}I,$$

where $Q_0 = I$.

3 An example

In this section, we illustrate Theorem 1 and Remark 2 by an example. Let

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0.8 & 0.2 & 0 \\ 0.4 & 0 & 0.2 & 0.4 \\ 0 & 0 & 0.25 & 0.75 \end{bmatrix}.$$

By (4),

$$L = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 0.2 & -0.2 & 0 \\ -0.4 & 0 & 0.8 & -0.4 \\ 0 & 0 & -0.25 & 0.25 \end{bmatrix}.$$

First, let us obtain the matrix $M$ of the mean first passage times by the direct use of (3). Finding

$$\pi = (0.08, 0.4, 0.2, 0.32)$$

and

$$L^\# = \begin{bmatrix} 0.7408 & 1.704 & -0.448 & -1.9968 \\ -0.1792 & 2.104 & -0.248 & -1.6768 \\ 0.2208 & -0.896 & 0.752 & -0.0768 \\ -0.0992 & -2.496 & -0.048 & 2.6432 \end{bmatrix}$$

and substituting these in (3) yields

$$M = \begin{bmatrix} 12.5 & 1 & 6 & 14.5 \\ 11.5 & 2.5 & 5 & 13.5 \\ 6.5 & 7.5 & 5 & 8.5 \\ 10.5 & 11.5 & 4 & 3.125 \end{bmatrix}.$$
Mention that one method to calculate $L^\#$ is by applying

$$L^\# = (L + \bar{J})^{-1} - \bar{J},$$

where

$$\bar{J} = (1, 1, \ldots, 1)^{\top} \pi.$$

(see, e.g., [2, (i) of Proposition 15]).

Now let us obtain $M$ by means of Theorem [1]. The weighted digraph $G$ corresponding to the Markov chain is shown in Fig. [1]. The converging trees of $G$ are shown in Fig. [2] where the roots are given in a boldface font.

\begin{figure}[h]
\centering
\begin{tabular}{|c|c|}
\hline
$1$ & $2$ \\
\hline
$3$ & $2$ \\
\hline
$4$ & $3$ \\
\hline
\end{tabular}
\end{figure}

Figure 1: The weighted digraph corresponding to the Markov chain.

\begin{figure}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$1$ & $2$ & $3$ & $4$ \\
\hline
$T_1$ & $T_2$ & $T_3$ & $T_4$ \\
\hline
$w(T_1) = 0.02$ & $w(T_2) = 0.1$ & $w(T_3) = 0.05$ & $w(T_4) = 0.08$ \\
\hline
\end{tabular}
\end{figure}

Figure 2: The converging trees $T_1, T_2, T_3,$ and $T_4$ of $G$.

By the definition of $q_i$ given in Theorem [1] one finds

$$q = (q_1, q_2, q_3, q_4) = (0.02, 0.1, 0.05, 0.08).$$

(17)

Since $\sum_{k=1}^4 q_i = 0.25$, by (17) it follows that

$$\bar{q} = (\bar{q}_1, \bar{q}_2, \bar{q}_3, \bar{q}_4) = \frac{q}{\sum_{k=1}^4 q_i} = (0.08, 0.4, 0.2, 0.32).$$

(18)
This vector coincides with $\pi$, the normalized left Perron vector of $T$.

The 2-tree in-forests of $G$ are presented in Fig. 3; the roots are shown there in a boldface font.

Figure 3: The 2-tree in-forests $F_1, \ldots, F_8$ of $G$.

In Theorem 1, $f_{ij}$ is defined as the total weight of 2-tree in-forests of $G$ that have one tree containing $i$ and the other tree converging to $j$. Therefore,

\[
(f_{ij}) = \begin{bmatrix}
0 & w(\{F_3\}) & w(\{F_2, F_5\}) & w(\{F_1, F_4, F_6, F_7, F_8\}) \\
w(\{F_2, F_3, F_7\}) & 0 & w(\{F_6\}) & w(\{F_1, F_4, F_6, F_8\}) \\
w(\{F_2, F_7\}) & w(\{F_3, F_5, F_8\}) & 0 & w(\{F_1, F_4, F_6\}) \\
w(\{F_1, F_2, F_7\}) & w(\{F_3, F_4, F_5, F_8\}) & w(\{F_6\}) & 0
\end{bmatrix}
\]

\[= \begin{bmatrix}
0 & 0.1 & 0.3 & 1.16 \\
0.23 & 0 & 0.25 & 1.08 \\
0.13 & 0.75 & 0 & 0.68 \\
0.21 & 1.15 & 0.2 & 0
\end{bmatrix},
\]

where $w(A)$ is the weight of a set of digraphs $A$. 

\[
(19)
\]
Substituting (17)–(19) in (11) yields the matrix of the mean first passage times:

\[
M = \begin{bmatrix}
12.5 & 1 & 6 & 14.5 \\
11.5 & 2.5 & 5 & 13.5 \\
6.5 & 7.5 & 5 & 8.5 \\
10.5 & 11.5 & 4 & 3.125
\end{bmatrix}.
\] (20)

Remark 2 enables one to avoid generating the converging trees and 2-tree in-forests of \( G \) shown in Fig. 2 and Fig. 3. Instead, \( f_{ij} \) and \( q_j \) can be computed by means of the recurrence procedure (12)–(13). Starting with \( Q_0 = I \), for example under consideration we have:

\[
\begin{align*}
\sigma_1 & = \frac{\text{tr}(LQ_0)}{1} = 2.25, \\
Q_1 & = -LQ_0 + \sigma_1 I = \begin{bmatrix}
1.25 & 1 & 0 & 0 \\
0 & 2.05 & 0.2 & 0 \\
0.4 & 0 & 1.45 & 0.4 \\
0 & 0 & 0.25 & 2
\end{bmatrix}, \\
\sigma_2 & = \frac{\text{tr}(LQ_1)}{2} = 1.56, \\
Q_2 & = -LQ_1 + \sigma_2 I = \begin{bmatrix}
0.31 & 1.05 & 0.2 & 0 \\
0.08 & 1.15 & 0.25 & 0.08 \\
0.18 & 0.4 & 0.5 & 0.48 \\
0.1 & 0 & 0.3 & 1.16
\end{bmatrix}, \\
\sigma_3 & = \frac{\text{tr}(LQ_2)}{3} = 0.25, \\
Q_3 & = -LQ_2 + \sigma_3 I = \begin{bmatrix}
0.02 & 0.1 & 0.05 & 0.08 \\
0.02 & 0.1 & 0.05 & 0.08 \\
0.02 & 0.1 & 0.05 & 0.08 \\
0.02 & 0.1 & 0.05 & 0.08
\end{bmatrix}. \\
\end{align*}
\] (21)

Denoting \( Q_2 = (q_{ij}^{(2)})_{n \times n} \), by (8) we have \( f_{ij} = q_{jj}^{(2)} - q_{ij}^{(2)}, i, j = 1, \ldots, n \), hence, by (21),

\[
(f_{ij}) = \begin{bmatrix}
0 & 0.1 & 0.3 & 1.16 \\
0.23 & 0 & 0.25 & 1.08 \\
0.13 & 0.75 & 0 & 0.68 \\
0.21 & 1.15 & 0.2 & 0
\end{bmatrix}, 
\] (23)

which coincides with (19). Eq. (22) yields \( q = (0.02, 0.1, 0.05, 0.08) \), which coincides with (17). Thus, we obtain Theorem 1 provides the matrix (20) of the mean first passage times again.
References

[1] Catral, M., M. Neumann and J. Xu, *Proximity in group inverses of M-matrices and inverses of diagonally dominant M-matrices*, Linear Algebra and its Applications 409 (2005), pp. 32–50.

[2] Chebotarev, P. and R. Agaev, *Forest matrices around the Laplacian matrix*, Linear Algebra and its Applications 356 (2002), pp. 253–274.

[3] Freidlin, M. I. and A. D. Wentzell, “Random Perturbations of Dynamical Systems,” Springer, New York, 1984.

[4] Leighton, T. and R. L. Rivest, *The Markov chain tree theorem*, Computer Science Technical Report MIT/LCS/TM-249, Laboratory of Computer Science, MIT, Cambridge, Mass. (1983).

[5] Leighton, T. and R. L. Rivest, *Estimating a probability using finite memory*, IEEE Transactions on Information Theory 32 (1986), pp. 733–742.

[6] Meyer, Jr., C. D., *The role of the group generalized inverse in the theory of finite Markov chains*, SIAM Review 17 (1975), pp. 443–464.

[7] Wentzell, A. D. and M. I. Freidlin, *On small random perturbations of dynamical systems*, Russian Mathematical Surveys 25 (1970), pp. 1–55.

[8] Wentzell, A. D. and M. I. Freidlin, “Fluctuations in Dynamical Systems under Small Random Perturbations,” Nauka, Moscow, 1979, in Russian.