Mean First Passage Matrices & the Inverse M–Matrix Problem

Michael Neumann, University of Connecticut

DeKalb, Illinois, August 2009

Research supported by NSA Grant No. 06G–232.

Joint work with Nung–Sing (Raymond) Sze

Stationary Probabilities vs MFP Times

Throughout we shall be concerned with a **finite state discrete–time homogeneous ergodic Markov chain** $\mathcal{C}$ or Markov chain for short.

Let $T = (t_{i,j})$ be the transition matrix for the chain, viz.

$$T \geq 0 \quad \textbf{and} \quad \sum_{j=1}^{n} t_{i,j} = 1, \quad \textbf{for all } i = 1, \ldots, n.$$

The stationary distribution of the chain is the unique positive vector

$$\pi = [\pi_1, \ldots, \pi_n]^t, \quad \pi^t T = \pi^t, \quad \|\pi\|_1 = 1.$$

The stationary distribution vector gives us long–range information on the chain: If the states of the system are $\mathcal{S}_1, \ldots, \mathcal{S}_n$, then π_j tells us the long term probability of the occurrence of state $\mathcal{S}_j$, $j = 1, \ldots, n$.

Mean First Passage Times

The **mean first passage time from state $\mathcal{S}_i$ to state $\mathcal{S}_j$ is the expected number of time–steps for reaching state $\mathcal{S}_j$ for the first time, given that initially the chain was in state $\mathcal{S}_i$.**

Formally, for $1 \leq\leq i, j \leq n$:

$$m_{i,j} \;=\; E(F_{i,j}) \;=\; \sum_{k=1}^{\infty} kPr(F_{i,j} = k).$$

Here $F_{i,j}$ is the random variable representing the smallest number of time–steps for reaching state $\mathcal{S}_j$ for the first time, given that the system was initially in state $\mathcal{S}_i$.
That is:

$$F_{i,j} \;=\; \min\{\ell \geq 1 : X_\ell = \mathcal{S}_j | X_0 = \mathcal{S}_i\}.$$

The matrix $M = (m_{i,j})$ is called the *mean first passage* (MFP) *matrix* of the chain.

In contrast to the stationary distribution vector, the mean first passage times give us information about the short range behavior of the chain. For example, suppose that we go to a holiday destination and we find that it is raining. Our interest then is not the average number of rainy days vs sunny days throughout the year, but rather how long we can expect it to turn sunny, given that it is now raining ?

How to Obtain MFP Times ?

Meyer 1975, Theorem 3.3

The MFP matrix for a Markov chain on n states whose transition matrix is $T \in \mathbb{R}^{n,n}$ is the unique solution of the matrix equation:

$$AX = J - TX_{\mathrm{dg}}$$

and the solution is given by

$$M = \left[I - A^{\#} + JA^{\#}_{\mathrm{dg}}\right] \Pi^{-1},$$

where $A = I - T$, $A^{\#}$ *is the group generalized inverse of* A, $\pi \in \mathbb{R}^{n,n}$ is **stationary distribution vector for the chain**, and where $\Pi = \mathrm{dg}(\pi)$.

In particular (Meyer [1975], Cho & Meyer [2000], Ditzenbacher [1988]):

(i) $m_{i,i} = \frac{1}{\pi_i}$, **for all** $i = 1, \ldots, n$.

(ii) $m_{i,j} = \frac{A^{\#}_{j,j} - A^{\#}_{i,j}}{\pi_j}$, **for all** $i \neq j$.

(iii) $\overline{M}_j := [m_{1,j}, \ldots, m_{j-1,j}, m_{j+1,j} \ldots, m_{n,j}]^T = A_j^{-1} e$,
where A_j the the $(n-1) \times (n-1)$ principal submatrix of A obtained by deleting its j–th row and column.

- Already above A_j is a nonsingular row diagonally dominant M–matrix.
- But most suggestively:

Theorem: (Tetali [1994])

Let $T = (t_{i,j}) \in \mathbb{R}^{n,n}$ be a transition matrix for a Markov chain with $T_{\mathrm{dg}} = 0$. Let and $A = I - T$ and $\Pi_n = \mathrm{diag}(\pi_1, \ldots, \pi_{n-1})$. Then

$$(\Pi_n A_n)H \;=\; I_{n-1},$$

where $H \;=\; (h_{i,j})$ is given by:

$$\mathbf{h_{i,j}} \;=\; \begin{cases} m_{i,n} + m_{n,i}, & \text{if } i = j, \\ m_{i,n} + m_{n,j} - m_{i,j}, & \text{if } i \neq j, \end{cases}$$

and where $M = (m_{i,j})$ is the MFP matrix for the chain.

Connection Between MFP Problems and M–matrices, Continued

Note: $A_n \in \mathbb{R}^{n,n}$ is a row diagonally dominant M–matrix $\Rightarrow \Pi_n A_n$ is a row diagonally dominant M–matrix $\Rightarrow H^{-1} = \Pi_n A_n$ is a row diagonally dominant M–matrix.

Claim: H^{-1} is (also) a column diagonally dominant M–matrix.

Proof: Partition π as $\pi = [\bar{\pi}^t \ \pi_n]^t$, where $\bar{\pi} \in R^{n-1,n-1}$. Observe first that because $\pi^t A = 0$ and A is an M–matrix, we can write that:

$$\bar{\pi}^t A_n = -\pi_n [a_{n,1} \ldots a_{n,n-1}] \geq 0. \qquad \left(A = \begin{bmatrix} A_n & * \\ [a_{n,1} \ldots a_{n,n-1}] & * \end{bmatrix} \right)$$

But $\Pi_n A_n = H^{-1}$ and so:

$$e^t H^{-1} = e^t \Pi_n A_n = \bar{\pi}^t A_n \geq 0.$$

Towards a First Characterization for Being an MFP Matrix

We mentioned that if $\mathcal{C}$ is a Markov chain with a transition matrix $T \in \mathbb{R}^{n,n}$ and an MFP matrix $M \in \mathbb{R}^{n,n}$, then M satisfies uniquely the matrix relation

$$(I - T)M \;=\; J - TM_{\rm dg}.$$

According to Kemeny and Snell [1960], if M is the MFP matrix for some Markov chain, then the matrix

$$N := M - M_{\rm dg}$$

is **always invertible**. They show that in terms of M, T is given by:

$$T \;=\; I + (M_{\rm dg} - J)N^{-1}$$

This motivates our question of:

Definition: The Inverse MFP Matrix Problem

Given a positive matrix $M \in \mathbb{R}^{n,n}$. Then when is M the MFP matrix of some Markov chain T **?**

A First, Immediate, Characterization

Observation: Giving necessary and sufficient conditions for $M \gg 0$ to be an MFP matrix

Let $M \in \mathbb{R}^{n,n}$ be a positive matrix and set $N := M - M_{\text{diag}}$. Then M is the MFP matrix for some Markov chain $\mathcal{C}$ whose transition matrix is T if and only if N is invertible and

$$\hat{T} \;=\; I + (M_{\text{dg}} - J)N^{-1}$$

is a nonnegative, irreducible, and stochastic matrix. In this case, $T = \hat{T}$.

An corollary showing the structure of the entries of N^{-1} is the following:

Corollary:

Soppose that $N \in \mathbb{R}^{n,n}$ is a nonnegative invertible matrix with zero diagonal entries. Let $N^{-1} = (p_{i,j})$. Then $N = M - M_{\text{dg}}$ for some MFP matrix M of a Markov chain $\mathcal{C}$ on n states if and only if

$$\sum_{k=1}^{n} p_{i,k} > 0 \quad \text{and} \quad p_{i,j} \geq \frac{\sum_{k=1}^{n} p_{i,k} \sum_{k=1}^{n} p_{k,j}}{\sum_{1 \leq k,\ell \leq n} p_{k,\ell}}, \quad \text{for all} \quad i \neq j.$$

Towards a Second Characterization for Being an MFP Matrix

Given a positive matrix $M = (m_{i,j}) \in \mathbb{R}^{n,n}$, define the matrix $H = (h_{i,j}) \in \mathbb{R}^{n-1,n-1}$ by:

$$\mathbf{h_{i,j}} = \begin{cases} m_{i,n} + m_{n,i}, & \text{if } i = j, \\ m_{i,n} + m_{n,j} - m_{i,j}, & \text{if } i \neq j. \end{cases}$$

Let

$$P = [I_{n-1} \ \ -e] \in \mathbb{R}^{(n-1),n}.$$

Then one can check that

$$H = -P(M - M_{\text{dg}})P^t.$$

One can immediately show that a Tetali–type theorem holds here if M is assumed to be an MFP matrix, without the restriction that $T_{\text{dg}} = 0$.

Theorem:

Suppose that T is the transition matrix of a Markov chain $\mathcal{C}$ on n states with the MFP matrix $M = (m_{i,j})$ with the stationary vector $\pi = (\pi_1, \ldots, \pi_n)^t$. Let $A = I - T$ and set $\Pi = \text{diag}\,(\pi_1, \ldots, \pi_n)$. Then

$$(\Pi_n A_n)H = I.$$

Characterization of Inverse M–Matrices

We already saw that $H = -P(M - M_{\rm dg})P^t \in R^{n-1,n-1}$ derived from an MFP matrix $M \in R^{n,n}$ is not only the inverse of a row diagonally dominant M–matrix, but also of a column diagonally dominant M–matrix.

We are now ready for our main result:

Theorem:

Let $H \in \mathbb{R}^{(n-1),(n-1)}$. Then the following are equivalent:

(a) H is invertible, H^{-1} is an irreducible row and column diagonally dominant M–matrix, and

$$\text{trace}\left((I+J)H^{-1}\right) \;\le\; 1.$$

(b) There exists a Markov chain $\mathcal{C}$ on n states with transition matrix $T \in \mathbb{R}^{n,n}$ and a stationary vector $\pi = (\pi_1, \ldots, \pi_n)$ such that

$$(\Pi_n A_n)H \;=\; I,$$

where $A = I - T$ and $\Pi = \text{dg}(\pi)$.

(c) There exists an MFP matrix M of a Markov chain $\mathcal{C}$ such that

$$H \;=\; -P(M - M_{\rm dg})P^t.$$

Proof that (a) $\Rightarrow$ (b)

$$\operatorname{trace}\left(H^{-1}\right) \;<\; \operatorname{trace}\left(H^{-1}\right) + \operatorname{trace}\left(JH^{-1}\right) \;\leq\; \operatorname{trace}\left((I+J)H^{-1}\right) \;\leq\; 1.$$

Let $d_1, \ldots, d_{n-1}$ be the diagonal entries of H^{-1}. Then we see that

$$\sum_{i=1}^{n-1} d_i \;<\; 1.$$

We can now choose positive numbers $\pi_1, \ldots, \pi_n$, with $\sum_{j=1}^{n} \pi_j = 1$, such that

$$\pi_j \;\geq\; d_j, \quad \text{for } j = 1, \ldots, n-1.$$

Set $\pi = (\pi_1, \ldots, \pi_n)^t$, $\Pi := \operatorname{diag}(\pi_1, \ldots, \pi_n)$, and

$$\mathbf{T} \;:=\; \mathbf{I} - \mathbf{\Pi^{-1} P^t H^{-1} P} \;=\; \mathbf{I} - \mathbf{\Pi}^{-1} \begin{bmatrix} H^{-1} & -H^{-1}e \\ -e^t H^{-1} & e^t H^{-1} e \end{bmatrix}.$$

Then T is nonnegative, irreducible, $Te = e$, and $\pi^t T = \pi^t$. Thus T is a transition matrix for some Markov chain whose stationary distribution is the vector π. Furthermore, we have that $\Pi_n A_n = H^{-1}$, where $A = I - T$.

Main Corollary:

Suppose that $A = (a_{i,j}) \in \mathbb{R}^{n \times n}$. Then the following conditions are equivalent:

(a) A is invertible and A^{-1} is an irreducible row and column diagonally dominant M–matrix.

(b) There exists a Markov chain $\mathcal{C}$ on $n+1$ states, with an MFP matrix $M = (m_{i,j})$, and a constant $k > 0$ such that

$$a_{i,j} = \begin{cases} k\left(m_{i,n+1} + m_{n+1,i}\right), & \text{if} \quad i = j, \\ \\ k\left(m_{i,n+1} + m_{n+1,j} - m_{i,j}\right), & \text{if} \quad i \neq j. \end{cases}$$

Extending Also Fiedler's Results

In 1998 Fiedler characterized inverses of symmetric diagonally dominant M–matrices in terms of **resistive electrical networks**.

Theorem ([Fiedler 1998])

Let $B = (b_{i,j}) \in \mathbb{R}^{n,n}$ be a real $n \times n$ matrix. Then the following are equivalent.

(a) B is invertible and B^{-1} is an irreducible diagonally dominant symmetric M–matrix.

(b) There is a connected resistive network $\mathcal{N}(\mathcal{G})$ with $n+1$ nodes $1, \ldots, n+1$ such that the *effective resistances* $R_{i,j}$ satisfy

$$b_{i,j} = \frac{1}{2}[R_{i,n+1} + R_{n+1,j} - R_{i,j}], \quad i, j = 1, \ldots, n.$$

Remark: Here $R_{i,i} = 0$, for all $i = 1, \ldots, n$.

Extending Fiedler's Results Continued

With the connected resistive network $\mathcal{N}(\mathcal{G})$ one can associate a random walk using the probabilities:

$$t_{i,j} \;=\; \frac{c_{i,j}}{\sum_{k\in V} c_{i,k}}, \quad i,j = 1,\ldots,n+1,$$

where $c_{i,j}$ denotes the conductance between node i and node j in the resistive network.

To connect Fiedler's result with our work we need the following 1996 proposition due to Chandra, Raghavan, Ruzzo, Smolensky, and Tiwari:

Proposition: Chandra, Raghavan, Ruzzo, Smolensky, and Tiwari, [1996]

Suppose that $\mathcal{N}(\mathcal{G})$ is a connected resistive network. Set:

$$\hat{C} \;:=\; \sum_{(i,j)\in V\times V} c_{i,j}.$$

Then for any two distinct nodes $i,j \in V$,

$$2m_{i,j} \;=\; \hat{C}R_{i,j},$$

Completing the arguments

$$\text{With} \qquad k \;:=\; \frac{1}{\hat{C}}$$

we find that for $i \neq j$, i,j=1,. . . , n+1,

$$km_{i,j} \;=\; \frac{1}{2}R_{i,j}$$

and so for $i \neq j$, we have that from Fiedler's condition on the $a_{i,j}$'s that:

$$b_{i,j} \;=\; \frac{1}{2}\left(R_{i,n+1} + R_{n+1,j} - R_{i,j}\right) \;=\; k\left(m_{i,n+1} + m_{n+1,j} - m_{i,j}\right),$$

while for $i = j$ we see that

$$b_{i,i} \;=\; \frac{1}{2}\left(R_{i,n+1} + R_{n+1,i} - \underbrace{R_{i,i}}_{=\,0}\right) \;=\; k(m_{i,n+1} + m_{n+1,i}).$$

Hence Fiedler's conditions lead to satisfying the condition of our Main Corollary with $k = \hat{C}$. Moreover, we observe that since A is symmetric in Fieldler's assumptions, it is the inverse of a row and column diagonally dominant M–matrix.