

Group inverses of M-matrices and applications to finite Markov chains and Laplacians of graphs

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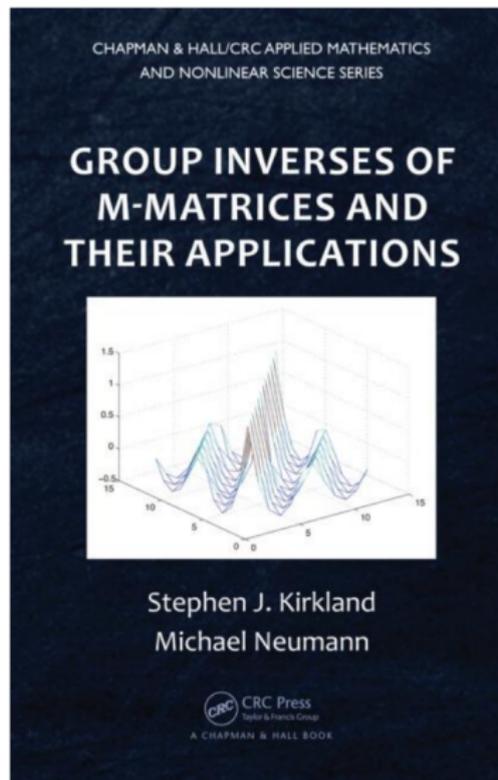
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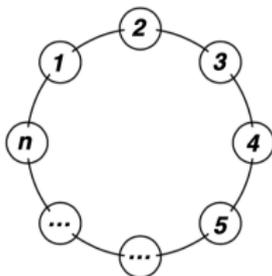
- ▶ M. Catral, M. Neumann and J. Xu. Proximity in group inverses of M -Matrices and inverses of diagonally dominant M -matrices, *Linear Algebra and Its Applications*, 409:32–50, 2005.
- ▶ M. Catral, M. Neumann and J. Xu. Matrix analysis of a Markov chain small-world model, *Linear Algebra and Its Applications*, 409:126–146, 2005.
- ▶ M. Catral, S.J. Kirkland, M. Neumann and N.-S. Sze. The Kemeny constant for finite homogeneous ergodic Markov chains, *Journal of Scientific Computing*, Volume 45, Numbers 1–3, 151–166, 2010.

References

- ▶ C. D. Meyer. The role of the group generalized inverse in the theory of finite Markov chains. *SIAM Rev.*, 17:443–464, 1975.

Example of a Markov chain model

Consider a ring network consisting of n nodes labeled as $1, \dots, n$, arranged in a clockwise manner with each node connected to its (nearest) neighboring nodes by undirected edges:



This defines an *ergodic* Markov chain representing a one-dimensional periodic random walk with transition matrix

$$T = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 & \dots & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \dots & 0 \\ 0 & \frac{1}{2} & 0 & \ddots & \dots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \dots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \frac{1}{2} & 0 \\ 0 & 0 & \ddots & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \dots & 0 & \frac{1}{2} & 0 \end{bmatrix} \in \mathbb{R}^{n,n}.$$

The matrix T is *irreducible* and *stochastic*.

A matrix $T \in \mathbb{R}^{n,n}$ is **irreducible** if it is not permutationally similar to a matrix of the form

$$\begin{bmatrix} A & B \\ 0 & C \end{bmatrix},$$

where $A \in \mathbb{R}^{k,k}$ for some $1 \leq k < n$.

The chain is **ergodic** \iff The transition matrix T is irreducible.
 \iff The directed graph of T is strongly connected.

Mean First Passage Matrix

Let $T \in \mathbb{R}^{n,n}$ be the transition matrix of a finite homogeneous ergodic Markov chain $\{X_k\}_{k=0}^{\infty}$ with states $\mathcal{S}_1, \dots, \mathcal{S}_n$.

- ▶ The **first passage time** from state \mathcal{S}_i to state \mathcal{S}_j is the random variable

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

the smallest value of ℓ such that the chain is in state \mathcal{S}_j after ℓ steps, given that the chain started in state \mathcal{S}_i .

- ▶ The **mean first passage time** from state \mathcal{S}_i to state \mathcal{S}_j is the expected value of F_{ij} :

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

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

Stationary Distribution Vector

The **stationary distribution vector** of the chain is the (positive) vector $\boldsymbol{\pi} = [\pi_1, \dots, \pi_n]^T$ satisfying

$$\boldsymbol{\pi}^T T = \boldsymbol{\pi}^T, \quad \|\boldsymbol{\pi}\|_1 = 1.$$

That is, $\boldsymbol{\pi}$ is the **left Perron vector** of T .

For example, if T is symmetric,

$$\boldsymbol{\pi} = \left[\frac{1}{n}, \dots, \frac{1}{n} \right]^T = \frac{1}{n} \mathbf{1}, \quad \text{where } \mathbf{1} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}.$$

Group Inverse

For $A \in \mathcal{R}^{n,n}$, the **group inverse**, if it exists, is the unique matrix X satisfying the matrix equations

$$AXA = A, \quad XAX = X \quad \text{and} \quad AX = XA.$$

If it exists, X is denoted by $A^\#$.

If A is nonsingular, $A^\# = A^{-1}$.

If A is singular, $A^\#$ exists $\Leftrightarrow 0$ is a *semisimple* eigenvalue of A .

$A^\#$ exists $\Leftrightarrow \text{rank } A = \text{rank } A^2$.

Spectral properties of the group inverse

For singular $A \in \mathcal{R}^{n,n}$ with group inverse $A^\# \in \mathcal{R}^{n,n}$, the following are true:

1. $A^\#$ has 0 as a semisimple eigenvalue and its multiplicity coincides with the multiplicity of 0 as an eigenvalue of A .
2. A vector \mathbf{x} is a right (resp. left) null vector for A if and only if it is a right (resp. left) null vector for $A^\#$.
3. The number $\lambda \neq 0$ is an eigenvalue of A of multiplicity m if and only if $1/\lambda$ is an eigenvalue of $A^\#$ of multiplicity m .
4. A vector \mathbf{x} is a right (resp. left) eigenvector for A corresponding to the eigenvalue $\lambda \neq 0$ if and only if it is a right (resp. left) eigenvector for $A^\#$ corresponding to the eigenvalue $1/\lambda$.

M-matrices

A matrix of the form $A = sI - B$, where $B \geq 0$ and $s \geq \rho(B)$ is called an **M-matrix**.

If $s > \rho(B)$, then $A = s \left(I - \frac{B}{s} \right) \Rightarrow$ (using the Neumann expansion)

$$A^{-1} = \frac{1}{s} \left(I + \frac{B}{s} + \frac{B^2}{s^2} + \dots \right).$$

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Theorem. A is a non-singular M-matrix if and only if A has non-positive off-diagonal entries and $A^{-1} \geq 0$.

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Theorem. A is a non-singular M-matrix if and only if A has non-positive off-diagonal entries and $A^{-1} \geq 0$.

Theorem. If A_1 and A_2 are non-singular M-matrices with $A_1 \leq A_2$, then $A_2^{-1} \leq A_1^{-1}$.

The M-matrix $A = I - T$

If T is the transition matrix of an n -state ergodic Markov chain, then $A = I - T$ is a singular M-matrix of rank $n - 1$.

Furthermore, the group inverse $A^\#$ exists and $A^\#$ *explains virtually everything that one would want to know about the Markov chain.*
(Meyer, 1975)

The group inverse associated with an M-matrix

Proposition. (Meyer 75) Let $T \in \mathcal{R}^{n,n}$ be an irreducible stochastic matrix and partition T as

$$T = \left[\begin{array}{c|c} T_{1,1} & T_{1,2} \\ \hline T_{2,1} & T_{2,2} \end{array} \right]$$

where $T_{1,1} \in \mathcal{R}^{n-1,n-1}$. Let $A = I - T$. Then $A^\#$ exists and can be written in partitioned form as

$$A^\# = (I - \mathbf{1}\pi^T) \left[\begin{array}{c|c} (I - T_{1,1})^{-1} & 0 \\ \hline 0 & 0 \end{array} \right] (I - \mathbf{1}\pi^T),$$

where $\mathbf{1} = [1, \dots, 1]^T$ and $\pi = [\pi_1, \dots, \pi_n]^T$ is the left Perron vector of T .

The group inverse associated with an M-matrix

Corollary. Let $T \in \mathcal{R}^{n,n}$ be an irreducible stochastic matrix and partition T as

$$T = \left[\begin{array}{c|c} T_{1,1} & T_{1,2} \\ \hline T_{2,1} & T_{2,2} \end{array} \right]$$

where $T_{1,1} \in \mathcal{R}^{n-1,n-1}$. Let $A = I - T$ and suppose that $A^\#$ is partitioned in conformity with the partitioning of T . Let $(A^\#)_{1,1} \in \mathbb{R}^{n-1,n-1}$ be the leading $(n-1) \times (n-1)$ principal submatrix of $A^\#$. Then

$$(A^\#)_{1,1} = A_n^{-1} + \beta W - A_n^{-1}W - WA_n^{-1},$$

where $A_n = I - T_{1,1}$, $\beta = \mathbf{u}^T A_n^{-1} \mathbf{1}$, $W = \mathbf{1} \mathbf{u}^T$, and $\boldsymbol{\pi}^T = [\mathbf{u}^T \ \pi_n]$ is the left Perron vector of T .

Mean first passage matrix and the group inverse of an associated M-matrix

Theorem. (Meyer 75) Let $T \in \mathcal{R}^{n,n}$ be the transition matrix of an n -state ergodic Markov chain with stationary distribution vector $\pi = [\pi_1, \dots, \pi_n]^T$ and mean first passage matrix $M = (m_{ij})$. Let $A = I - T$. Then

$$M = (I - A^\# + JA_d^\#)\Pi^{-1}$$

where

$$\begin{aligned} J &= \text{the } n \times n \text{ matrix of all } 1\text{'s}, \\ A_d^\# &= \text{diag}(A_{1,1}^\#, \dots, A_{n,n}^\#), \\ \Pi &= \text{diag}(\pi_1, \dots, \pi_n). \end{aligned}$$

Mean first passage matrix and the group inverse of an associated M-matrix

The proof uses the fact that the mean first passage matrix for the transition matrix T is the unique solution M to the matrix equation

$$M = T(M - M_{\text{dg}}) + J$$

where for any $n \times n$ matrix A , A_{dg} is defined as

$$A_{\text{dg}} = \text{diag}(a_{1,1}, \dots, a_{n,n})$$

where $a_{1,1}, \dots, a_{n,n}$ are the diagonal entries of A .

Observations.

1. Let $\boldsymbol{\pi} = [\pi_1, \dots, \pi_n]^T$, the stationary distribution vector of T .
Then

$$\begin{aligned}\boldsymbol{\pi}^T M &= \boldsymbol{\pi}^T (I - A^\# + J A_d^\#) \Pi^{-1} \\ &= (\boldsymbol{\pi}^T - \underbrace{\boldsymbol{\pi}^T A^\#}_{\mathbf{0}^T} + \underbrace{\boldsymbol{\pi}^T J A_d^\#}_{\mathbf{1}^T}) \Pi^{-1} \\ &= (\boldsymbol{\pi}^T + \mathbf{1}^T \text{diag}(A_{1,1}^\#, \dots, A_{n,n}^\#)) \text{diag}\left(\frac{1}{\pi_1}, \dots, \frac{1}{\pi_n}\right) \\ &= \mathbf{1}^T + \mathbf{1}^T \text{diag}\left(\frac{A_{1,1}^\#}{\pi_1}, \dots, \frac{A_{n,n}^\#}{\pi_n}\right).\end{aligned}$$

Thus, for $k = 1, \dots, n$,

$$(\boldsymbol{\pi}^T M)_k = 1 + \frac{A_{k,k}^\#}{\pi_k}.$$

Observations.

2. Let $M = (m_{i,j})$ be the mean first passage matrix for the transition matrix T . Since

$$M = (I - A^\# + JA_d^\#) \begin{pmatrix} \frac{1}{\pi_1} & & \\ & \ddots & \\ & & \frac{1}{\pi_n} \end{pmatrix},$$

the (i,j) -entry of M is

$$\begin{aligned} m_{i,j} &= \sum_{k=1}^n (I - A^\# + JA_d^\#)_{i,k} \delta_{k,j} \frac{1}{\pi_j} \\ &= \frac{A_{jj}^\# - A_{ij}^\#}{\pi_j}, \text{ if } i \neq j, \end{aligned}$$

and

$$m_{i,i} = \frac{1}{\pi_i}.$$

Relation between the mean first passage times and row sums of inverses of principal submatrices of singular M-matrices

Let $A = I - T$, where T is the transition matrix of an n -state ergodic Markov chain. For $j = 1, \dots, n$, let A_j be the $(n - 1) \times (n - 1)$ principal submatrix of A obtained by deleting its j th row and column. Then

- ▶ A_j is a nonsingular, irreducible and row diagonally dominant M-matrix.
- ▶ A_j^{-1} is a nonnegative matrix, so its row sums are nonnegative as well.

Relation between the mean first passage times and row sums of inverses of principal submatrices of singular M-matrices

Theorem. Let $A = I - T$, where T is the transition matrix of an n -state ergodic Markov chain with mean first passage matrix $M = (m_{i,j})$. For $j = 1, \dots, n$, let

$$\bar{M}_j = [m_{1,j}, \dots, m_{j-1,j}, m_{j+1,j}, \dots, m_{n,j}]^T$$

(that is \bar{M}_j is the j -th column of M with the j -th entry deleted).
Then

$$\bar{M}_j = A_j^{-1} \mathbf{1},$$

where A_j is the $(n-1) \times (n-1)$ principal submatrix of A obtained by deleting its j th row and column, and $\mathbf{1}$ is the $(n-1)$ -vector of all ones.

Relation between the mean first passage times and row sums of inverses of principal submatrices of singular M-matrices

Theorem. Let $A = I - T$, where T is the transition matrix of an n -state ergodic Markov chain with mean first passage matrix $M = (m_{ij})$. For $j = 1, \dots, n$, with $i \neq j$,

$$m_{ij} = (A_j^{-1} \mathbf{1})_i = \sum_{t=1}^{n-1} (A_j^{-1})_{i,t}$$

where A_j is the $(n-1) \times (n-1)$ principal submatrix of A obtained by deleting its j th row and column, and $\mathbf{1}$ is the $(n-1)$ -vector of all ones.

The Kemeny Constant

Let $i \in \{1, \dots, n\}$ be fixed and let

$$K_i = \sum_{j=1}^n m_{i,j} \pi_j.$$

Then K_i gives the mean first passage time from state \mathcal{S}_i when the destination state is unknown.

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Then K_i gives the mean first passage time from state \mathcal{S}_i when the destination state is unknown.

Theorem. [Kemeny-Snell, Hunter, ...]

$$K_i = K, \quad \text{for all } i.$$

The number K is called **Kemeny's constant**.

Kemeny's constant measures the expected number of steps from any initial state to a randomly chosen final state, and is thus regarded as an indicator of the overall transit efficiency of the corresponding Markov chain. (Xu-Kirkland 2019)

The Kemeny Constant

Theorem. $K = 1 + \text{trace}(A^\#)$.

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Theorem. $K = 1 + \text{trace}(A^\#)$.

Proof: Using mean first passage matrix in terms of group inverse,

$$m_{i,j} = \begin{cases} \frac{A_{j,j}^\# - A_{i,j}^\#}{\pi_j} & , \text{ if } i \neq j, \\ \frac{1}{\pi_j} & , \text{ if } i = j. \end{cases}$$

Thus,

$$\begin{aligned} K &= \sum_{j=1}^n m_{i,j} \pi_j = 1 + \text{trace}(A^\#) - A_{i,i}^\# - \sum_{j \neq i} A_{i,j}^\# \\ &= 1 + \text{trace}(A^\#) - \underbrace{\sum_{j=1}^n A_{i,j}^\#}_0, \end{aligned}$$

since $\mathbf{1}$ is a null vector for $A = I - T$.

The Kemeny Constant

Corollary.

$$K = 1 + \sum_{i=2}^n \frac{1}{1 - \lambda_i},$$

where $\lambda_2, \dots, \lambda_n$ are the eigenvalues of T other than 1.

Another formula for Kemeny constant

Theorem. For $j = 1, \dots, n$

$$K = 1 + \text{trace}(A_j^{-1}) - \frac{A_{j,j}^\#}{\pi_j},$$

where A_j is the $(n-1) \times (n-1)$ principal submatrix of A obtained by deleting its j th row and column.

Proof: Without loss of generality, assume $j = n$.

For $i, j = 1, \dots, n-1$, $i \neq j$,

1. $m_{i,j}\pi_j = A_{j,j}^\# - A_{i,j}^\#$,
2. $A_{i,j}^\# = (A_n^{-1})_{i,j} + \beta\pi_j - (A_n^{-1}\mathbf{1})_i\pi_j - \sum_{k=1}^{n-1} \pi_k (A_n^{-1})_{k,j}$,
3. $A_{j,j}^\# = (A_n^{-1})_{j,j} + \beta\pi_j - (A_n^{-1}\mathbf{1})_j\pi_j - \sum_{k=1}^{n-1} \pi_k (A_n^{-1})_{k,j}$.

Proceed by performing the algebra. □

Note the observation

$$(\pi^T M)_j = 1 + \frac{A_{j,j}^\#}{\pi_j}$$

implies

$$\frac{A_{j,j}^\#}{\pi_j} = \sum_{k \neq j} \pi_k m_{k,j}.$$

So,

$$\frac{A_{j,j}^\#}{\pi_j} \approx \text{(weighted) average of the mean first passage times into state } j \text{ from any other state.}$$

Effect of perturbation

Question. Suppose that the matrix T of transition probabilities is perturbed by adding an error matrix E such that the resulting matrix $\bar{T} = T + E$ is still irreducible and stochastic. How would such a perturbation affect the new Kemeny constant \bar{K} ?

Perturbation example

Let

$$T = \begin{bmatrix} t_{1,1} & t_{1,2} & \cdots & \cdots & t_{1,n} \\ t_{2,1} & t_{2,2} & \cdots & \cdots & t_{2,n} \\ \vdots & \vdots & & & \vdots \\ t_{n,1} & t_{n,2} & \cdots & \cdots & t_{n,n} \end{bmatrix}$$

and suppose that

$$\begin{aligned} \bar{T} &= T + \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} [h_1 \ \cdots \ h_n] \\ &= T + \mathbf{1}\mathbf{h}^T, \quad \mathbf{1} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}, \quad \mathbf{h} = \begin{bmatrix} h_1 \\ \vdots \\ h_n \end{bmatrix}, \\ &\quad \text{and } \mathbf{h}^T \mathbf{1} = 0. \end{aligned}$$

Theorem. If T and \bar{T} are as above with respective Kemeny constants K and \bar{K} , then $\bar{K} = K$.

Proof. Follows from $K = 1 + \sum_{i=2}^n \frac{1}{1 - \lambda_i}$,

where $\lambda_2, \dots, \lambda_n$ are the eigenvalues of T other than 1, and the fact that T and \bar{T} have the same eigenvalues.

Corollary If $\mathbf{h} = \varepsilon(\mathbf{e}_i - \mathbf{e}_j)$, then

$$\frac{\overline{A}_{j,j}^\#}{\overline{\pi}_j} \geq \frac{A_{j,j}^\#}{\pi_j},$$

and

$$\frac{\overline{A}_{i,i}^\#}{\overline{\pi}_i} \leq \frac{A_{i,i}^\#}{\pi_i}.$$

Proof. (First part) Follows from

$$\begin{aligned} K &= 1 + \text{trace}(A_j^{-1}) - \frac{A_{j,j}^\#}{\pi_j}, \\ \overline{K} &= 1 + \text{trace}(\overline{A}_j^{-1}) - \frac{\overline{A}_{j,j}^\#}{\overline{\pi}_j}, \end{aligned}$$

and the fact that A_j and \overline{A}_j are non-singular M-matrices with $\overline{A}_j \leq A_j$.

Theorem Let T be a symmetric, stochastic and irreducible matrix, and suppose that $\bar{T} = T + E$, where E is a positive semi-definite matrix such that \bar{T} remains stochastic and irreducible. Let $K = K(T)$ and $\bar{K} = K(\bar{T})$ be their respective Kemeny constants. Then $K \leq \bar{K}$.

Theorem Let T be a symmetric, stochastic and irreducible matrix, and suppose that $\bar{T} = T + E$, where E is a positive semi-definite matrix such that \bar{T} remains stochastic and irreducible. Let $K = K(T)$ and $\bar{K} = K(\bar{T})$ be their respective Kemeny constants. Then $K \leq \bar{K}$.

Proof: Let λ_i and $\bar{\lambda}_i$, $i = 2, \dots, n$, be the eigenvalues of T and \bar{T} respectively, that are different from 1. Then by Weyl's Theorem,

$$\lambda_i \leq \bar{\lambda}_i, \quad i = 2, \dots, n.$$

Thus,

$$\sum_{i=2}^n \frac{1}{1 - \lambda_i} \leq \sum_{i=2}^n \frac{1}{1 - \bar{\lambda}_i},$$

and hence, $K \leq \bar{K}$. □

Example

Consider an ergodic Markov chain representing a one-dimensional periodic random walk with transition matrix

$$T = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}.$$

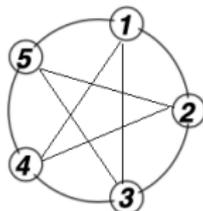
Perturb T by adding the following positive semi-definite error matrix E :

$$E = \begin{bmatrix} 0.0954 & -0.0395 & 0.0285 & 0.0127 & -0.0971 \\ -0.0395 & 0.0524 & -0.0479 & 0.0116 & 0.0234 \\ 0.0285 & -0.0479 & 0.0705 & -0.0573 & 0.0063 \\ 0.0127 & 0.0116 & -0.0573 & 0.0922 & -0.0591 \\ -0.0971 & 0.0234 & 0.0063 & -0.0591 & 0.1265 \end{bmatrix}.$$

The resulting matrix $\bar{T} = T + E$ is

$$\bar{T} = \begin{bmatrix} 0.0954 & 0.4605 & 0.0285 & 0.0127 & 0.4029 \\ 0.4605 & 0.0524 & 0.4521 & 0.0116 & 0.0234 \\ 0.0285 & 0.4521 & 0.0705 & 0.4427 & 0.0063 \\ 0.0127 & 0.0116 & 0.4427 & 0.0922 & 0.4409 \\ 0.4029 & 0.0234 & 0.0063 & 0.4409 & 0.1265 \end{bmatrix},$$

which is still irreducible and stochastic.



A perturbation of the Markov Chain

“Short-cuts” are added to non-neighboring nodes.

Then, by previous theorem, $K \leq \bar{K}$. That is, the average of the mean first passage times from any state will not decrease.

Proximity in Group Inverses of M-matrices

Let $\mathcal{G} = (V, E)$ be a connected undirected weighted graph with vertex set $V = \{1, \dots, n\}$ and edge set E . With \mathcal{G} we can associate the *Laplacian matrix* $L = (\ell_{i,j}) \in \mathbb{R}^{n,n}$, whose entries are given by

$$\ell_{i,j} = \begin{cases} -w_{i,j}, & \text{if } i \neq j \text{ and } i \text{ is adjacent to } j \\ & \text{with an edge of weight } w_{i,j} \\ 0, & \text{if } i \neq j \text{ and} \\ & i \text{ is not adjacent to } j \\ -\sum_{k \neq i} \ell_{i,k}, & \text{if } i = j. \end{cases}$$

It is known that L is a symmetric, irreducible, positive semi-definite M-matrix of rank $n - 1$. Hence, $L^\#$ exists. Also, $I + L$ is a non-singular M-matrix.

Proximity between vertices of a graph

- ▶ The problem of evaluating the *proximity* (distance) between vertices of a graph was studied by Chebotarev and Shamis [1997].
- ▶ The main vehicle is the derivation of certain properties of the matrix $Q = (I + L)^{-1} = (q_{i,j})$, where L is the Laplacian matrix of the graph.
- ▶ The entry $q_{i,j}$ is interpreted as the fraction of connectivity of the vertices i and j with respect to the total connectivity of i with all the vertices in the graph.

Theorem. (Chebotarev and Shamis [1996]): Let $Q = (I + L)^{-1} = (q_{i,j})$. Then for all $1 \leq i, j, k \leq n$,

$$q_{i,i} - q_{j,i} - q_{i,k} + q_{j,k} \geq 0. \quad (*)$$

(*) is called the **triangle inequality for proximities**.

Remark:

Let

$$\begin{aligned} d_{i,j} &= q_{i,i} + q_{j,j} - q_{i,j} - \underbrace{q_{j,i}}_{=q_{i,j}} \\ &= q_{i,i} + q_{j,j} - 2q_{i,j}. \end{aligned}$$

Then d is a *metric* on the set of vertices of \mathcal{G} .

We can generalize (*) as follows:

Theorem Let $T \in \mathbb{R}^{n,n}$ be nonnegative, irreducible and stochastic, and let $\boldsymbol{\pi} = [\pi_1, \dots, \pi_n]^T$, $\|\boldsymbol{\pi}\|_1 = 1$, be its normalized left Perron vector. Let $A = I - T$. Then for any $1 \leq i, j, k \leq n$,

$$\frac{A_{i,j}^\#}{\pi_j} - \frac{A_{j,i}^\#}{\pi_i} - \frac{A_{i,k}^\#}{\pi_k} + \frac{A_{j,k}^\#}{\pi_k} \geq 0.$$

We can generalize (*) as follows:

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$$\frac{A_{i,j}^\#}{\pi_j} - \frac{A_{j,i}^\#}{\pi_i} - \frac{A_{i,k}^\#}{\pi_k} + \frac{A_{j,k}^\#}{\pi_k} \geq 0.$$

Proof:

(1) Triangular Inequality for Mean First Passage Times (Hunter [2002])

$$m_{i,j} \leq m_{i,k} + m_{k,j}.$$

(2) Mean first passage matrix in terms of group inverse

$$m_{i,j} = \begin{cases} \frac{A_{j,j}^\# - A_{i,j}^\#}{\pi_j} & , \text{ if } i \neq j, \\ \frac{1}{\pi_j} & , \text{ if } i = j. \end{cases}$$

Special Cases

- ▶ If T is symmetric, then $\boldsymbol{\pi} = \left[\frac{1}{n}, \dots, \frac{1}{n}\right]^T$, i.e., $\pi_j = \frac{1}{n}$, for all j .

In this case,

$$A_{i,i}^{\#} - A_{j,i}^{\#} - A_{i,k}^{\#} + A_{j,k}^{\#} \geq 0,$$

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Special Cases

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- ▶ For the Laplacian Matrix:

$$L = D - W,$$

where

W = weight matrix

D = $\text{diag}(d_i)$, where $d_i = \sum_{j \neq i} w_{i,j}$.

Let $d = \max_{1 \leq i \leq n} d_i > 0$. Then

$$L = dI - B,$$

where

$$B = \text{diag}(d - d_i) + W \geq 0$$

and

$$\rho(B) = \|B\|_\infty = d.$$

Hence, we can write

$$L = d(I - T),$$

where $T = \frac{1}{d}B$ is stochastic and irreducible.

Thus,

$$L_{i,i}^\# - L_{j,i}^\# - L_{i,k}^\# + L_{j,k}^\# \geq 0,$$

for $1 \leq i, j, k \leq n$.

Generalization of CS Proximity Theorem

Theorem Let $A \in \mathbb{R}^{n,n}$ be a non-singular, irreducible, symmetric and row diagonally-dominant M-matrix. Let $B = A^{-1} = (b_{i,j})$. Then for all $1 \leq i, j, k \leq n$,

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Idea of proof:

Embed A in a singular, irreducible, symmetric M-matrix F with zero row sums:

$$F = \left[\begin{array}{c|c} A & F_{1,2} \\ \hline F_{2,1} & F_{2,2} \end{array} \right] \in \mathbb{R}^{n+1,n+1}$$

where $F_{1,2}^T = F_{2,1}$, $A\mathbf{1} + F_{1,2} = 0$, $F_{2,1}\mathbf{1} + F_{2,2} = 0$, and $\mathbf{1} = [1 \cdots 1]^T$.

Then

$$F_{i,i}^{\#} - F_{j,i}^{\#} - F_{i,k}^{\#} + F_{j,k}^{\#} \geq 0,$$

for all $1 \leq i, j, k \leq n+1$.

Let $(F^\#)_{1,1}$ = the leading $n \times n$ principal submatrix of $F^\#$.

Q. How is $(F^\#)_{1,1}$ related to A^{-1} ?

Meyer [1975]:

$$\begin{aligned} \underbrace{(F^\#)_{1,1}}_{n \times n} &= A^{-1} + \frac{\sigma}{n+1} J - \frac{1}{n+1} (A^{-1} J + J A^{-1}) \\ &= B + \frac{\sigma}{n+1} J - \frac{1}{n+1} (B J + J B), \end{aligned}$$

where $\sigma = \mathbf{1}^T A^{-1} \mathbf{1} / (n+1)$.

Hence, for $i, j, k = 1, \dots, n$:

$$F_{i,i}^\# - F_{j,i}^\# - F_{i,k}^\# + F_{j,k}^\# = b_{i,i} - b_{j,i} - b_{i,k} + b_{j,k} \geq 0.$$

Applications to the Perron root function

The Perron-Frobenius Theorems.

Let $A \in \mathbb{R}^{n,n}$ be a nonnegative and irreducible matrix, and let $r = \rho(A)$. Then

1. $r > 0$ and r is a simple eigenvalue of A .
2. A has a positive eigenvector corresponding to the eigenvalue r .
3. If $0 \leq B \leq A$, then $\rho(B) \leq \rho(A)$. Equality holds $\iff A = B$.

The eigenvalue $r = \rho(A)$ is called the **Perron root** of A .

Applications to the Perron root function

Let T be a nonnegative and irreducible matrix. Then $A = \rho(T)I - T$ is a singular and irreducible M -matrix with a group inverse $A^\#$.

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For a function f of a matrix B , the notation $\frac{\partial f(B)}{\partial_{i,j}}$ denotes the partial derivative with respect to the (i,j) th entry of B .

Theorem. (Deutsch, Neumann [1984]). Let T be a nonnegative and irreducible matrix, and $A = \rho(T)I - T$. Let $\mathbf{u} = [u_1, \dots, u_n]^T$ and $\mathbf{v} = [v_1, \dots, v_n]^T$ be the right and left Perron vectors of T (i.e., $T\mathbf{u} = \rho(T)\mathbf{u}$ and $\mathbf{v}^T T = \rho(T)\mathbf{v}^T$), normalized so that $\mathbf{v}^T \mathbf{u} = 1$. Then

$$\frac{\partial^2 \rho(T)}{\partial_{i,j}^2} = 2v_i u_j A_{j,i}^\#.$$

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$$\frac{\partial^2 \rho(T)}{\partial_{i,j}^2} = 2v_i u_j A_{j,i}^\#.$$

Question. When is the Perron root a concave function of every off-diagonal entry?

The question above is equivalent to:
If A is a singular and irreducible M -matrix, when is $A^\#$ an M -matrix?

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Theorem. The following conditions are equivalent for $A \in \mathbb{R}^{n,n}$:

(1) A is an M -matrix.

(2) All the off-diagonal entries of A are nonpositive, and all of the principal minors of A are nonnegative.

Mohan, Neumann, Ramamurthy [1984] :

If A is a singular irreducible M -matrix, then all of the principal minors of $A^\#$ are nonnegative.

So, it is left to tackle the sign patterns of the off-diagonal entries of $A^\#$.

Question: For $i \neq j$, when is $A_{i,j}^\# \leq 0$?

When is $A_{i,j}^{\#} \leq 0$?

Theorem Let $T \in \mathbb{R}^{n,n}$ be nonnegative, irreducible and stochastic and let $\boldsymbol{\pi} = [\pi_1, \dots, \pi_n]^T$, $\|\boldsymbol{\pi}\|_1 = 1$, be the normalized left Perron vector of T . Suppose that $A = I - T$ and $M = (m_{i,j})$ is the mean first passage matrix for the finite homogeneous ergodic Markov chain whose transition matrix is T . Then for any pair (i,j) with $i \neq j$ and $1 \leq i, j \leq n$,

$$A_{i,j}^{\#} \leq 0 \iff m_{i,j} \geq \sum_{k \neq j} \pi_k m_{k,j}.$$

When is $A_{i,j}^{\#} \leq 0$?

Theorem Let $T \in \mathbb{R}^{n,n}$ be nonnegative, irreducible and stochastic and let $\boldsymbol{\pi} = [\pi_1, \dots, \pi_n]^T$, $\|\boldsymbol{\pi}\|_1 = 1$, be the normalized left Perron vector of T . Suppose that $A = I - T$ and $M = (m_{i,j})$ is the mean first passage matrix for the finite homogeneous ergodic Markov chain whose transition matrix is T . Then for any pair (i,j) with $i \neq j$ and $1 \leq i, j \leq n$,

$$A_{i,j}^{\#} \leq 0 \iff m_{i,j} \geq \sum_{k \neq j} \pi_k m_{k,j}.$$

Proof:

$$A_{i,j}^{\#} \leq 0 \iff m_{i,j} \geq \frac{A_{j,j}^{\#} - A_{i,j}^{\#}}{\pi_j} \geq \frac{A_{j,j}^{\#}}{\pi_j}.$$

When is $A_{i,j}^{\#} \leq 0$?

We can use the two different representations for mean first passage times to derive a correspondence involving the maximum row sum of the inverse of a deleted submatrix A_j and the minimum entry in the j th column of the group inverse of A .

When is $A_{i;j}^\# \leq 0$?

Theorem Let $T \in \mathbb{R}^{n,n}$ be nonnegative, irreducible and stochastic and let $\boldsymbol{\pi} = [\pi_1, \dots, \pi_n]^T$, $\|\boldsymbol{\pi}\|_1 = 1$, be the normalized left Perron vector of T . Let $A = I - T$. For each $j = 1, \dots, n$, let A_j be the $(n-1) \times (n-1)$ principal submatrix of A obtained by deleting the j -th row and column of A . For each $\ell = 1, \dots, n-1$, let

$$r_\ell^{(j)} = \sum_{t=1}^{n-1} (A_j^{-1})_{\ell,t}. \quad (1)$$

(That is, $r_\ell^{(j)} = A_j^{-1} \mathbf{1}$, the ℓ -th row sum of A_j^{-1} .)

Let $1 \leq i \leq n$ with $i \neq j$. Then $A_{i;j}^\# \leq 0$ if and only if

$$r_k^{(j)} \geq \sum_{s=1}^{j-1} \pi_s r_s^{(j)} + \sum_{s=j}^{n-1} \pi_{j+1} r_s^{(j)}, \quad (2)$$

where

$$k = \begin{cases} i, & \text{if } 1 \leq i < j \\ i-1, & \text{if } j < i \leq n. \end{cases} \quad (3)$$

In particular, suppose that $1 \leq k \leq n - 1$ is an index for which

$$\sum_{\nu=1}^{n-1} (A_j^{-1})_{k,\nu} = \max_{1 \leq \nu \leq n-1} \sum_{\nu=1}^{n-1} (A_j^{-1})_{\mu,\nu} = \|A_j^{-1}\|_{\infty}.$$

Then $A_{p,j}^{\#} < 0$, where

$$p = \begin{cases} k, & \text{if } 1 \leq k < j \\ k + 1, & \text{if } j \leq k \leq n - 1. \end{cases} \quad (4)$$

Examples

Consider an ergodic Markov chain representing a one-dimensional periodic random walk with transition matrix

$$T = \begin{bmatrix} 0 & 0.5 & 0 & 0 & 0.5 \\ 0.5 & 0 & 0.5 & 0 & 0 \\ 0 & 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0.5 & 0 & 0.5 \\ 0.5 & 0 & 0 & 0.5 & 0 \end{bmatrix}.$$

and let

$$A = I - T = \begin{bmatrix} 1 & -0.5 & 0 & 0 & -0.5 \\ -0.5 & 1 & -0.5 & 0 & 0 \\ 0 & -0.5 & 1 & -0.5 & 0 \\ 0 & 0 & -0.5 & 1 & -0.5 \\ -0.5 & 0 & 0 & -0.5 & 1 \end{bmatrix}.$$

Then the group inverse $A^\#$ of A is given by

$$A^\# = \begin{bmatrix} 0.8 & 0 & -0.4 & -0.4 & 0 \\ 0 & 0.8 & 0 & -0.4 & -0.4 \\ -0.4 & 0 & 0.8 & 0 & -0.4 \\ -0.4 & -0.4 & 0 & 0.8 & 0 \\ 0 & -0.4 & -0.4 & 0 & 0.8 \end{bmatrix}.$$

Examples

The group inverse $A^\#$

$$A^\# = \begin{bmatrix} 0.8 & 0 & -0.4 & -0.4 & 0 \\ 0 & 0.8 & 0 & -0.4 & -0.4 \\ -0.4 & 0 & 0.8 & 0 & -0.4 \\ -0.4 & -0.4 & 0 & 0.8 & 0 \\ 0 & -0.4 & -0.4 & 0 & 0.8 \end{bmatrix}$$

is an M-matrix.

The mean first passage matrix for the finite ergodic homogeneous Markov chain with transition matrix T is

$$M = \begin{bmatrix} 5 & 4 & 6 & 6 & 4 \\ 4 & 5 & 4 & 6 & 6 \\ 6 & 4 & 5 & 4 & 6 \\ 6 & 6 & 4 & 5 & 4 \\ 4 & 6 & 6 & 4 & 5 \end{bmatrix}.$$

Note that the right side of the condition

$$A_{i,j}^\# \leq 0 \iff m_{i,j} \geq \sum_{k \neq j} \pi_k m_{k,j}.$$

is in this case equivalent to: $m_{i,j} \geq \frac{1}{5} \sum_{k \neq j} m_{k,j}$.

References

References

- ▶ M. Catral, M. Neumann and J. Xu. Proximity in group inverses of M -Matrices and inverses of diagonally dominant M -matrices, *Linear Algebra and Its Applications*, 409:32–50, 2005.
- ▶ M. Catral, M. Neumann and J. Xu. Matrix analysis of a Markov chain small-world model, *Linear Algebra and Its Applications*, 409:126–146, 2005.
- ▶ M. Catral, S.J. Kirkland, M. Neumann and N.-S. Sze. The Kemeny constant for finite homogeneous ergodic Markov chains, *Journal of Scientific Computing*, Volume 45, Numbers 1–3, 151–166, 2010.

References

- ▶ C. D. Meyer. The role of the group generalized inverse in the theory of finite Markov chains. *SIAM Rev.*, 17:443–464, 1975.

Thank You!