The Role of Generalized Matrix Inverses in Markov Chains

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1. Introduction

Let $P = [p_{ij}]$ be the transition matrix of a finite irreducible, discrete time Markov chain (MC) $\{X_n\}$ $(n \geq 0)$ with finite state space $S = \{1, 2, \ldots, m\}$.

$$i.e.\ \ p_{ij} = P\{X_n = j \mid X_{n-1} = i\} \text{ for all } i, j \in S.$$

Such MCs have a unique stationary distribution

$$\{\pi_j\},\ (1 \leq j \leq m).$$

Let T_{ij} be the first passage time RV from state i to state j,

i.e. T_{ij} = min{ $n \geq 1$ such that $X_n = j$ given that $X_0 = i$}.

T_{ii} is the first return to state i.

Let $m_{ij} = E[T_{ij} \mid X_0 = i]$,

be the mean first passage time from state i to state j.

Generalized matrix inverses (g-inverses) of $I-P$ are typically used to solve systems of linear equations to deduce expressions for $\{\pi_j\}$ and the $\{m_{ij}\}$, either in matrix form or in terms of the elements of the g-inverse.

Further, the elements of every g-inverse of $I-P$ can be expressed in terms of the $\{\pi_j\}$ and the $\{m_{ij}\}$ of the associated MC.

2. Generalized Matrix Inverses

A generalized inverse of a matrix A is any matrix A^{-} such that $AA^{-}A = A$.

A^{-} is a "one condition" g-inverse, $A^{(1)}$

A^{-} is an "equation solving" g-inverse

If A is non-singular, $A^{-} = A^{-1}$, the inverse of A, and is unique. In general A^{-} is not unique.

Multi-condition g-inverses:

Consider real conformable matrices X (which we assume to be square)

Condition 1: $AXA = A$

Condition 2: $XAX = X$

Condition 3: $(AX)^{T} = AX$

Condition 4: $(XA)^{T} = XA$

Condition 5: $AX = XA$

Let $A^{(i,j,\,.\,.)}$ be any $(i,j,\,.\,.)$ condition g-inverse of A then

$A^{(1,2)}$ is a "pseudo-inverse" (Rao, 1955)
is a "reciprocal inverse" (Bjerhammar, 1951)
is a "reflexive inverse" (Rhode, 1964)

$A^{(1,3)}$ is a "least squares g-inverse"

$A^{(1,4)}$ is a "minimum norm g-inverse"

$A^{(1,2,4)}$ is a "weak generalized inverse"
(Goldman & Zelen, 1964)

$A^{(1,2,3,4)}$ is the "Moore-Penrose g-inverse"
(Moore, 1920; Penrose, 1955)

$A^{(1,2,5)}$ is the "group Inverse"
(exists and is unique if $r(A) = r(A^2)$.)
(Erdeyli,1967)

3. Solving systems of linear equations

A necessary and sufficient condition for

$$AXB = C$$

to have a solution is

$$AA^{-} CB^{-} B = C.$$

If this consistency condition is satisfied, the general solution is given by

$$X = A^{-}CB^{-} + W - A^{-}AWBB^{-}$$

where W is an arbitrary matrix.

(Penrose 1955, Rao,1955)

Special cases

(i) The general solution of $XB = C$ *is*

$$X = CB^{-} + W(I - BB^{-}) \text{ provided } CB^{-}B = C,$$

where W is arbitrary.

(ii) The general solution of $AX = C$ is

$$X = A^{-}C + (I - A^{-}A)W \text{ provided } AA^{-}C = C,$$

where W is arbitrary.

(iii) The general solution of $AXA = A$ is

$$X = A^{-}AA^{-} + W - A^{-}AWAA^{-},$$

where W is arbitrary, (since $AA^{-}AA^{-}A = AA^{-}A = A$.)

Note that (iii) provides a characterization of $A\{1\}$,
the set of all g-inverses of A given any one g-inverse, A^{-} :

$$A\{1\} = \{A^{-} + H - A^{-}AHAA^{-} , \ H \text{ arbitrary}\}$$

or

$$A\{1\} = \{A^{-} + (I - A^{-}A)F + G(I - AA^{-}), \ F, \ G, \text{ arbitrary}\}.$$

4. G-inverses of Markovian kernels, *I* – *P*

Let P be the transition matrix of a finite irreducible Markov chain with stationary probability vector $\boldsymbol{\pi}^T$.

Let $\mathbf{e}^T = (1, 1, \ldots, 1)$ and $\boldsymbol{t}$ and $\boldsymbol{u}$ be any vectors.

$I - P + \boldsymbol{t}\boldsymbol{u}^T$ is non-singular

$\Leftrightarrow\ \boldsymbol{\pi}^T\boldsymbol{t} \neq 0$ and $\boldsymbol{u}^T\mathbf{e} \neq 0$.

If $\boldsymbol{\pi}^T\boldsymbol{t} \neq 0$ and $\boldsymbol{u}^T\mathbf{e} \neq 0$ then

$[I - P + \boldsymbol{t}\boldsymbol{u}^T]^{-1}$ is a g-inverse of $I - P$.

(Hunter, 1982)

All one condition g-inverses of $I - P$ can be expressed as

$$A^{(1)} = [I - P + \boldsymbol{t}\boldsymbol{u}^T]^{-1} + \boldsymbol{e}\boldsymbol{f}^T + \boldsymbol{g}\boldsymbol{\pi}^T$$

where $\boldsymbol{f}$, $\boldsymbol{g}$, $\boldsymbol{t}$, and $\boldsymbol{u}$ are arbitrary with $\boldsymbol{u}^T\boldsymbol{e} \neq 0$ and $\boldsymbol{\pi}^T\boldsymbol{t} \neq 0$.

(Hunter, 1982)

Given any g-inverse G of $I - P$ and $\boldsymbol{t}$, $\boldsymbol{u}$, with $\boldsymbol{\pi}^T\boldsymbol{t} \neq 0$, $\boldsymbol{u}^T\boldsymbol{e} \neq 0$, we can compute $[I - P + \boldsymbol{t}\boldsymbol{u}^T]^{-1}$ as

$$[I - P + \boldsymbol{t}\boldsymbol{u}^T]^{-1} = \left[I - \frac{\boldsymbol{e}\boldsymbol{u}^T}{\boldsymbol{u}^T\boldsymbol{e}}\right] G \left[I - \frac{\boldsymbol{t}\boldsymbol{\pi}^T}{\boldsymbol{\pi}^T\boldsymbol{t}}\right] + \frac{\boldsymbol{e}\boldsymbol{u}^T}{(\boldsymbol{\pi}^T\boldsymbol{t})(\boldsymbol{u}^T\boldsymbol{e})}.$$

(Hunter, 1988)

Parametric characterisation of g-inverses of I - P

(Hunter, 1990)

If G is any g-inverse of $I - P$ there exist unique parameters $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and γ such that

$$G = G(\boldsymbol{\alpha}, \boldsymbol{\beta}, \gamma) = [\mathrm{I} - P + \boldsymbol{\alpha}\boldsymbol{\beta}^T]^{-1} + \gamma \mathbf{e}\boldsymbol{\pi}^T,$$

with the property that $\boldsymbol{\alpha}, \boldsymbol{\beta}$ and γ involve 2m – 1 independent parameters with the properties that

$$\boldsymbol{\pi}^T\boldsymbol{\alpha} = 1,\ \boldsymbol{\beta}^T\mathbf{e} = 1 \text{ and } \gamma + 1 = \boldsymbol{\beta}^T G\boldsymbol{\alpha}.$$

Construction of the unique characterisation

Given G, any g-inverse of $I - P$,

Let $A \equiv I - (I - P)G$ and $B \equiv I - G(I - P)$.

Then $A = \boldsymbol{\alpha\pi}^T$, $B = \mathbf{e}\boldsymbol{\beta}$, and

$$G = [I - P + \boldsymbol{\alpha\beta}^T]^{-1} + \gamma\mathbf{e}\boldsymbol{\pi}^T,$$

where $\boldsymbol{\alpha} = A\mathbf{e}$,

$$\boldsymbol{\beta}^T = \boldsymbol{\pi}^T B \ (= \mathbf{e}_i^T B \text{ for all } i),$$

and $\gamma + 1 = \boldsymbol{\pi}^T G\boldsymbol{\alpha} = \boldsymbol{\beta}^T G\mathbf{e} = \boldsymbol{\beta}^T G\boldsymbol{\alpha}.$

$\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, γ uniquely characterise the g-inverse as G($\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, γ).

Application:

Let $G = G(\alpha, \beta, \gamma)$ be a (α, β, γ) g-inverse of $I - P$.

$G \in A\{1,\ 2\} \Leftrightarrow \gamma = -1.$

$G \in A\{1,\ 3\} \Leftrightarrow \boldsymbol{\alpha} = \boldsymbol{\pi} / \boldsymbol{\pi}^T\boldsymbol{\pi}.$

$G \in A\{1,\ 4\} \Leftrightarrow \boldsymbol{\beta} = \mathbf{e}^T / \mathbf{e}^T\mathbf{e}.$

$G \in A\{1,\ 5\} \Leftrightarrow \boldsymbol{\alpha} = \mathbf{e},\ \boldsymbol{\beta}^T = \boldsymbol{\pi}^T.$

We subdivide the A{1,5} category:

$G \in A\{1,\ 5a\} \Leftrightarrow \boldsymbol{\alpha} = \mathbf{e},$

$G \in A\{1,\ 5b\} \Leftrightarrow \boldsymbol{\beta}^T = \boldsymbol{\pi}^T.$

so that

$G \in A\{1,\ 5\} \Leftrightarrow G \in A\{1,\ 5a\}$ and $G \in A\{1,\ 5b\}.$

Theorem

Let $G = G(\boldsymbol{\alpha}, \boldsymbol{\beta}, \gamma)$ be a $(\boldsymbol{\alpha}, \boldsymbol{\beta}, \gamma)$ g-inverse of $I - P$, where P is the transition matrix of a finite irreducible MC with stationary probability vector $\boldsymbol{\pi}$.

(a) G $\in$ A{1, 5*a*} $\Leftrightarrow$ G$\mathbf{e}$ = $g\mathbf{e}$ for some g.

If G$\mathbf{e}$ = $g\mathbf{e}$ for some g then g = 1 + γ.

(b) G $\in$ A{1, 5b} $\Leftrightarrow \boldsymbol{\pi}^T G = h\boldsymbol{\pi}^T$ for some h

If $\boldsymbol{\pi}^T G = h\boldsymbol{\pi}^T$ for some h then h = 1 + γ

Corollary:

Let $G = G(\boldsymbol{\alpha}, \boldsymbol{\beta}, \gamma)$ be a $(\boldsymbol{\alpha}, \boldsymbol{\beta}, \gamma)$ g-inverse of $I - P$.

If G$\mathbf{e}$ = $g\mathbf{e}$ for some g and $\boldsymbol{\pi}^T G = h\boldsymbol{\pi}^T$ for some h

then g = h = 1 + γ and G $\in$ A{1, 5}. i.e. $G = G(\mathbf{e}, \boldsymbol{\pi}, \gamma)$.

Special cases of g-inverses of I – P

(a) $Z = [I - P + \Pi]^{-1}$ where $\Pi = \mathbf{e}\boldsymbol{\pi}^T$

(Kemeny & Snell's fundamental matrix, Z, 1960)

Shown to be a 1-condition g-inverse, Hunter (1969).

Z is a (1,5) g-inverse with form $G = G(\mathbf{e}, \boldsymbol{\pi}, 0)$.

(b) $A^{\#} = [I - P + \mathbf{e}\boldsymbol{\pi}^T]^{-1} - \mathbf{e}\boldsymbol{\pi}^T = Z - \Pi$ (Group inverse)

(Meyer, 1975)

$A^{\#}$ is the unique (1, 2, 5) g-inverse with form $G = G(\mathbf{e}, \boldsymbol{\pi}, -1)$.

Special cases of g-inverses of I – P

(c) $G = G(\boldsymbol{\pi} / \boldsymbol{\pi}^T \boldsymbol{\pi}, \mathbf{e}/\mathbf{e}^T \mathbf{e}, -1)$ is the Moore-Penrose g-inverse

$$G = [I - P + \alpha \boldsymbol{\pi} \mathbf{e}^T]^{-1} - \alpha \Pi \text{ where } \alpha = (m \boldsymbol{\pi}^T \boldsymbol{\pi})^{-1/2}$$

(Styan, Paige, Wachter, 1975)

Alternative form: $G = [I - P + \boldsymbol{\pi} \mathbf{e}^T]^{-1} - \dfrac{\mathbf{e}\boldsymbol{\pi}^T}{m \boldsymbol{\pi}^T \boldsymbol{\pi}}.$

Equivalence comes from the fact that

$$A_\delta = [I - P + \delta \boldsymbol{t}\boldsymbol{u}^T]^{-1} - \frac{\mathbf{e}\boldsymbol{\pi}^T}{\delta(\boldsymbol{\pi}^T \boldsymbol{t})(\boldsymbol{u}^T \mathbf{e})} \text{ does not depend on } \delta.$$

(Hunter, 1988)

5. Stationary distributions

Finite irreducible MC's $\{X_n\}$ have a unique stationary distribution $\{\pi_j\},(1 \le j \le m)$ which, for aperiodic MC's is the limiting distribution,

$$i.e. \lim_{n\to\infty} P\{X_n = j \mid X_0 = i\} = \lim_{n\to\infty} P\{X_n = j\} = \pi_j, (1 \le j \le m).$$

Let $\boldsymbol{\pi}^T = (\pi_1, \pi_2, \ldots, \pi_m)$ be the stationary prob. vector for the irreducible MC with transition matrix $P = [p_{ij}]$.

We need to solve $\pi_j = \sum_{i=1}^{m} \pi_i p_{ij}$ with $\sum_{i=1}^{m} \pi_i = 1$,

i.e. $\boldsymbol{\pi}^T (I - P) = 0^T$ with $\boldsymbol{\pi}^T \mathbf{e} = 1$.

This is an equation of the type $XB = C$,

with $X = \boldsymbol{\pi}^T, B = I - P, C = \boldsymbol{0}^T$.

Procedures using $A = I - (I - P)G$

If G is any g-inverse of $I - P$ and $A = I - (I - P)G$ then

$$\pi^T = \frac{\boldsymbol{v}^T A}{\boldsymbol{v}^T A\boldsymbol{e}},$$

where $\boldsymbol{v}^T$ is such that $\mathbf{v}^T A\boldsymbol{e} \neq 0$.

Note: $A\boldsymbol{e} \neq 0$ so that we can always find such a $\boldsymbol{v}^T$.

Procedure using $A = I - (I - P)G$

Let G be any g-inverse of $I - P$, and $A = I - (I - P)G = [a_{ij}]$.

Let r be the smallest integer i $(1 \le i \le m)$ such that $\sum_{k=1}^{m} a_{ik} \ne 0$,

then $\pi_j = \dfrac{a_{rj}}{\sum_{k=1}^{m} a_{rk}}, \ j = 1, \ldots, m.$

If G is a (1,3) or (1,5) g-inverse of $I - P$ then r = 1.

Procedures using *G*

If $G = [I - P + \boldsymbol{t}\boldsymbol{u}^T]^{-1}$ where $\boldsymbol{u}$, $\boldsymbol{t}$ such that $\boldsymbol{u}^T\mathrm{e} \neq 0$, $\boldsymbol{\pi}^T\boldsymbol{t} \neq 0$,

$$\boldsymbol{\pi}^T = \frac{\boldsymbol{u}^T G}{\boldsymbol{u}^T G\mathbf{e}}.$$

(Paige, Styan, Wachter,1975),
(Kemeny,1981), (Hunter,1982).

If G is a (1,4) g-inverse of $I - P$ then

$$\boldsymbol{\pi}^T = \frac{\mathbf{e}^T G}{\mathbf{e}^T G\mathbf{e}}.$$

Special g-inverses of form $G = [I - P + \boldsymbol{tu}^T]^{-1}$

Identifier	g-inverse	Parameters		
	$[I - P + \boldsymbol{tu}^T]^{-1}$	$\boldsymbol{\alpha}$	$\boldsymbol{\beta}^T$	γ
G_{ee}	$[I - P + \boldsymbol{ee}^T]^{-1}$	$\boldsymbol{e}$	$\boldsymbol{e}^T/m$	$(1/m) - 1$
$G_{eb}^{(r)}$	$[I - P + \boldsymbol{e}\,\boldsymbol{p}_b^{(r)T}]^{-1}$	$\boldsymbol{e}$	$\boldsymbol{p}_b^{(r)T}$	0
G_{eb}	$[I - P + \boldsymbol{e}\,\boldsymbol{e}_b^T]^{-1}$	$\boldsymbol{e}$	$\boldsymbol{e}_b^T$	0
$G_{ae}^{(c)}$	$[I - P + \boldsymbol{p}_a^{(c)}\boldsymbol{e}^T]^{-1}$	$\boldsymbol{p}_a^{(c)}/\pi_a$	$\boldsymbol{e}^T/m$	$(1/m\pi_a) - 1$
$G_{ab}^{(c,r)}$	$[I - P + \boldsymbol{p}_a^{(c)}\boldsymbol{p}_b^{(r)T}]^{-1}$	$\boldsymbol{p}_a^{(c)}/\pi_a$	$\boldsymbol{p}_b^{(r)T}$	$(1/\pi_a) - 1$
$G_{ab}^{(c)}$	$[I - P + \boldsymbol{p}_a^{(c)}\boldsymbol{e}_b^T]^{-1}$	$\boldsymbol{p}_a^{(c)}/\pi_a$	$\boldsymbol{e}_b^T$	$(1/\pi_a) - 1$
G_{ae}	$[I - P + \boldsymbol{e}_a\boldsymbol{e}^T]^{-1}$	$\boldsymbol{e}_a/\pi_a$	$\boldsymbol{e}^T/m$	$(1/m\pi_a) - 1$
$G_{ab}^{(r)}$	$[I - P + \boldsymbol{e}_a\boldsymbol{p}_b^{(r)T}]^{-1}$	$\boldsymbol{e}_a/\pi_a$	$\boldsymbol{p}_b^{(r)T}$	$(1/\pi_a) - 1$
G_{ab}	$[I - P + \boldsymbol{e}_a\boldsymbol{e}_b^T]^{-1}$	$\boldsymbol{e}_a/\pi_a$	$\boldsymbol{e}_b^T$	$(1/\pi_a) - 1$
$G_{tb}^{(c)}$	$[I - P + \boldsymbol{t}_b\boldsymbol{e}_b^T]^{-1}$ $(\boldsymbol{t}_b \equiv \boldsymbol{e} - \boldsymbol{e}_b + \boldsymbol{p}_b^{(c)})$	$\boldsymbol{t}_b$	$\boldsymbol{e}_b^T$	0

Special case: $G = [I - P + \boldsymbol{eu}^T]^{-1}$ (with $\boldsymbol{u}^T\boldsymbol{e} \neq 0$).

$$\boldsymbol{\pi}^T = \boldsymbol{u}^T G,$$

Hence if $\boldsymbol{u}^T = (u_1, u_2, \ldots, u_m)$ and $G = [g_{ij}]$ then

$$\pi_j = \sum_{k=1}^{m} u_k g_{kj},\ j = 1, 2, \ldots, m.$$

Thus $G_{ee} = [I - P + \boldsymbol{ee}^T]^{-1} \Rightarrow \pi_j = \sum_{k=1}^{m} g_{kj} = g_{\bullet j}$

$$G_{eb}^{(r)} = [I - P + \boldsymbol{ep}_b^{(r)T}]^{-1} \Rightarrow \pi_j = \sum_{k=1}^{m} p_{bk} g_{kj}$$

$$G_{eb} = [I - P + \boldsymbol{ee}_b^T]^{-1} \Rightarrow \pi_j = g_{bj}$$

Special case: $G = [I - P + \boldsymbol{t}\mathbf{e}^T]^{-1}$ (with $\boldsymbol{\pi}^T\mathbf{e} \neq 0$).

$$\boldsymbol{\pi}^T = \frac{\mathbf{e}^T G}{\mathbf{e}^T G \mathbf{e}}.$$

Hence if $G = [g_{ij}]$ then

$$\pi_j = \frac{g_{\bullet j}}{g_{\bullet\bullet}}, j = 1, 2, \ldots, m.$$

Holds for $G_{ae}^{(c)} = [I - P + \boldsymbol{p}_a^{(c)}\mathbf{e}^T]^{-1}$,

$$G_{ee} = [I - P + \mathbf{e}\mathbf{e}^T]^{-1} \quad (\Rightarrow \pi_j = g_{\bullet j}),$$

$$G_{ae} = [I - P + \mathbf{e}_a\mathbf{e}^T]^{-1}.$$

Special case: $G = [I - P + \boldsymbol{t}\mathbf{e}_b^T]^{-1}$ (with $\boldsymbol{\pi}^T\mathbf{e} \neq 0$).

$$\boldsymbol{\pi}^T = \frac{\mathbf{e}_b^T G}{\mathbf{e}_b^T G\mathbf{e}},$$

Hence if $G = [g_{ij}]$ then

$$\pi_j = \frac{g_{bj}}{g_{b\bullet}}, j = 1, 2, ..., m.$$

Holds for $G_{ab}^{(c)} = [I - P + \boldsymbol{p}_a^{(c)}\mathbf{e}_b^T]^{-1}$,

$$G_{ab} = [I - P + \mathbf{e}_a\mathbf{e}_b^T]^{-1},$$

$$G_{eb} = [I - P + \mathbf{e}\mathbf{e}_b^T]^{-1} \quad (\Rightarrow \pi_j = g_{bj}),$$

$$G_{tb}^{(c)} = [I - P + \boldsymbol{t}_b\mathbf{e}_b^T]^{-1} \quad (\Rightarrow \pi_j = g_{bj}).$$

6. Moments of first passage time distributions

Let T_{ij} be the **first passage time** RV from state *i* to state *j*,

$\{X_n\}$ irreducible $\Rightarrow$ T_{ij} are proper r.v.'s.

For all i, j $\in$ S, and $k \geq 1$ let $m_{ij}^{(k)} = E[T_{ij}^k \mid X_0 = i]$.

The $m_{ij}^{(k)}$ are well defined and finite.

Let $m_{ij}^{(1)} = m_{ij}$, the mean first passge time from state *i* to state *j*.

Let $M = [m_{ij}]$ be the matrix of mean first passage times

Let $M^{(2)} = [m_{ij}^{(2)}]$ be the matrix of second moments.

Well known that

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

M satisfies the matrix equation

$$(I - P)M = E - PM_d,$$

where E = [1] = $\boldsymbol{ee}^T$,

and $M_d = [\delta_{ij} m_{ij}] = (\Pi_d)^{-1} \equiv D$ (with $\Pi = \boldsymbol{e\pi}^T$).

i.e. equation of the type $AX = C$, where
$X = M$, $A = I - P$ and C = $E - PD$.

If G is any g-inverse of $I - P$, then

$$M = [G\Pi - E(G\Pi)_d + I - G + EG_d]D.$$

(Hunter, 1982)

Thus if $G = [g_{ij}]$, and $g_{i\bullet} = \sum_{j=1}^{m} g_{ij}$, then

$$m_{ij} = \frac{[g_{jj} - g_{ij} + \delta_{ij}]}{\pi_j} + (g_{i\bullet} - g_{j\bullet}), \text{ for all } i, j.$$

Joint computation for π_j and m_{ij}

1. Compute $G = [g_{ij}]$, ANY g-inverse of $I - P$.
2. Compute sequentially rows 1, 2, …r ($\leq$ m) of

   $A = I - (I - P)G \equiv [a_{ij}]$ until $\sum_{k=1}^{m} a_{rk}$, (1$\leq$ r $\leq$ m)

   is the first non-zero sum.
3. Compute $\pi_j = a_{rj} \Big/ \sum_{k=1}^{m} a_{rk}, \quad j = 1, \ldots, m.$
4. Compute $m_{jj} = \sum_{k=1}^{m} a_{rk} \Big/ a_{rj}$, $j = 1, \ldots, m$, and for, $i \neq j$.

   $$m_{ij} = \left\{ (g_{jj} - g_{ij}) \sum_{k=1}^{m} a_{rk} \Big/ a_{rj} \right\} + \left\{ \sum_{k=1}^{m} (g_{ik} - g_{jk}) \right\}.$$

Let $H = G(I - \Pi)$ then

$M = [I - H + EH_d]D.$

H leads to simpler elemental forms for M:

$$\text{If } H = [h_{ij}],\ m_{ij} = \frac{[h_{jj} - h_{ij} + \delta_{ij}]}{\pi_j},\ \text{for all } i, j,$$

$$\text{i.e. } m_{ij} = \begin{cases} \dfrac{1}{\pi_j} & i = j, \\[2ex] \dfrac{(h_{jj} - h_{ij})}{\pi_j}, & i \neq j. \end{cases}$$

We can simplify this further under special conditions:

Theorem: $G \in A\{1, 5a\} \Leftrightarrow M = [I - G + EG_d]D.$

Thus under any of the following equivalent conditions:

(i) $G \in A\{1, 5a\}$

(ii) $G\mathbf{e} = g\mathbf{e}$, g a constant,

(iii) $GE - E(G\Pi)_d D = 0$,

(iv) $G\Pi - E(G\Pi)_d = 0$,

we have that $M = [I - G + EG_d]D$ and

$$m_{ij} = \frac{[g_{jj} - g_{ij} + \delta_{ij}]}{\pi_j}, \text{ for all } i, j,$$

Significance of H = G(I – Π)

Let $G = G(\boldsymbol{\alpha}, \boldsymbol{\beta}, \gamma)$ be any 1 - condition g-inverse of $I - P$,

Then $H = G(I - \Pi)$ is a g-inverse of $I - P$ with

$$H = G(\mathbf{e}, \boldsymbol{\beta}, -1) \in A\{1, 2, 5a\}.$$

Further $K = (I - \Pi)H = (I - \Pi)G(I - \Pi)$ is a g-inverse of $I - P$

with $K = G(\mathbf{e}, \boldsymbol{\pi}, -1) \in A\{1, 2, 5\}$, the group inverse.

Special cases with the simple elemental form for the m_{ij} :

(a) $G = [I - P + \Pi]^{-1} = Z$ where $\Pi = \mathbf{e}\boldsymbol{\pi}^T$

Kemeny & Snell's fundamental matrix ($\gamma = 0$)

(Kemeny and Snell, 1960)

(b) $G = [I - P + \Pi]^{-1} - \Pi = Z - \Pi = A^{\#}$

Meyer's Group inverse ($\gamma = -1$) (Meyer, 1975)

Second moments of the first passage times

$M^{(2)}$ satisfies the matrix equation

$$(I-P)M^{(2)} = E + 2P(M - M_d) - PM_d^{(2)}.$$

where $M_d^{(2)} = 2D(\Pi M)_d - D,$ with $D = M_d = (\Pi_d)^{-1}.$

G is any g-inverse of $I-P$, $M_d^{(2)} = D + 2D\{(I-\Pi)G(I-\Pi)\}_d D.$

$G \in A\{1,5a\} \Rightarrow M_d^{(2)} = D + 2DG_dD - 2D(\Pi G)_d D,$

$G \in A\{1,5b\} \Rightarrow M_d^{(2)} = D + 2DG_dD - 2D(G\Pi)_d D,$

$G \in A\{1,5\} \Rightarrow M_d^{(2)} = 2DG_dD - (1+2\gamma)D,$

In particular, $M_d^{(2)} = D + 2DA_d^{\#}D = 2DZ_dD - D.$

Second moments of first passage times

If G is any g-inverse of $I - P$,

$$M^{(2)} = 2[GM - E(GM)_d] + [I - G + EG_d][M_d^{(2)} + D] - M,$$
$$= 2[GM - E(GM)_d] + 2[I - G + EG_d]D(\Pi M)_d - M.$$

If $G \in A(1, 5a)$ then

$$M^{(2)} = 2[GM - E(GM)_d] + MD^{-1}M_d^{(2)}.$$

In particular,

$$M^{(2)} = 2[ZM - E(ZM)_d] + M(2Z_d D - I),$$
$$= 2[A^{\#}M - E(A^{\#}M)_d] + M(2A_d^{\#}D + I).$$

(Hunter, 2007b)

Elemental expressions for $m_{ij}^{(2)}$

If $G = [g_{ij}]$ then

$$m_{ij}^{(2)} = 2\sum_{k=1}^{m}(g_{ik} - g_{jk})m_{kj} - m_{ij} + (\delta_{ij} - g_{ij} + g_{jj})(m_{jj}^{(2)} + m_{jj}).$$

If $G\mathbf{e} = g\mathbf{e} \Leftrightarrow G \in A(1,5a)$, then

$$m_{ij}^{(2)} = 2\sum_{k=1}^{m}(g_{ik} - g_{jk})m_{kj} + \frac{m_{ij}m_{jj}^{(2)}}{m_{jj}}.$$

$$m_{jj}^{(2)} + m_{jj} = 2m_{jj}\sum_{i=1}^{m}\pi_i m_{ij}.$$

(Hunter, 2007b)

Computational considerations - 1

Two relevant papers:

[1] Heyman and O'Leary (1995) ("Computations with Markov chains" (2nd International Workshop on M.C.'s)

[2] Heyman and Reeves (1989) (ORSA J Computing)

[1]: "deriving means and variances of first passage times from either the fundamental matrix Z or the group generalized inverse $A^{\#}$ leads to a significant inaccuracy on the more difficult problems."

… "it does not make sense to compute either the fundamental matrix or the group generalized inverse unless the individual elements of those matrices are of interest."

Computational considerations - 2

[2]: Computation of M using Z or $A^{\#}$ - 3 sources of error

1. An algorithm for computing π.
2. Compute the inverse of $I - P + \Pi$.
   (Matrix may have negative elements - can cause round off-errors in computing inverse.)
3. Matrix evaluation of M - the matrix multiplying D may have negative elements.

Additional work to compute $M^{(2)}$ - three matrix multiplications are required - two of which involve a diagonal matrix - in each of these multiplications there is a matrix with possibly negative elements.

There has to be a better way!

Simpler computation technique

Let $G_{eb} = [g_{ij}] = [I - P + \mathbf{e}\mathbf{e}_b^T]^{-1}$ (a special A(1, 5a) g-inverse)

$$\pi_j = g_{bj},\ j = 1,2,\ldots,m;\ \ m_{ij} = \frac{\delta_{ij} + g_{jj} - g_{ij}}{g_{bj}} = \begin{cases} 1/g_{bj}, & i = j, \\ (g_{jj} - g_{ij})/g_{bj}, & i \neq j. \end{cases}$$

Thus following one matrix inversion (actually only the *b*-th row for the stationary distribution), one can find the stationary probabilities and the mean first passage times.

$$m_{ij}^{(2)} = \begin{cases} m_{jj}[1 + 2m_{jj}(g_{jj} - g_{bj}^{(2)})], & i = j, \\ 2m_{jj}[g_{jj}^{(2)} - g_{ij}^{(2)} + m_{ij}(g_{jj} - g_{bj}^{(2)})] - m_{ij}, & i \neq j. \end{cases}$$

$$var[T_{ij}] = \begin{cases} m_{jj}[1 - m_{jj} + 2m_{jj}(g_{jj} - g_{bj}^{(2)})], & i = j, \\ 2m_{jj}[g_{jj}^{(2)} - g_{ij}^{(2)} + m_{ij}(g_{jj} - g_{bj}^{(2)})] - m_{ij}(1 - m_{ij}), & i \neq j. \end{cases}$$

7. G-inverses in terms of stationary probabilities and mean first passage times

Let $G = G(\alpha, \beta, \gamma)$ be any 1-condition g-inverse of $I - P$

then, since $G\alpha = (\gamma + 1)\mathbf{e}$ and $\beta^T G = (\gamma + 1)\boldsymbol{\pi}^T$,

(i) $$g_{jj} = \frac{1}{\alpha_j}\left(1 + \gamma - \sum_{k \neq j} \alpha_k g_{jk}\right).$$

(ii) $$g_{jj} = \frac{1}{\beta_j}\left((1 + \gamma)\pi_j - \sum_{i \neq j} \beta_i g_{ij}\right).$$

If we have expressions for the g_{ij} when $i \neq j$ we can deduce expressions for all the g_{jj}.

We do not, in general have any information from the previous results about $g_{i\bullet} = \sum_{j=1}^{m} g_{ij}$ for specific *i*.

If $\alpha_k = \alpha$, a constant (= 1, since $\boldsymbol{\pi}^T\boldsymbol{\alpha} = \alpha\boldsymbol{\pi}^T\mathbf{e} = \alpha$)

$\Rightarrow$ $g_{i\bullet} = 1 + \gamma$, *a* constant fo all *i*.

Thus when $\boldsymbol{\alpha}$ = **e**, i.e when G $\in$ A{1, 5a}

$$g_{ij} = g_{jj} + \pi_j m_{ij}, \text{ for all } i \neq j.$$

We explore the special case when $\boldsymbol{\alpha}$ = **e** later.

We need a procedure that yields expressions for $g_{i\bullet}$

Let $G = G(\alpha, \beta, \gamma)$ be any 1-condition g-inverse of I – P

Let $H = G(I - \Pi) \equiv [h_{ij}]$

h_{ij} can be expressed in terms of the $\{\beta_k\}$ parameters of the g-inverse.

If $\delta_j \equiv \sum_{k \neq j}^{m} \beta_k m_{kj}$, then

$$h_{jj} = \pi_j \delta_j \ (j = 1,2, ..m)$$

$$h_{ij} = \pi_j (\delta_j - m_{ij}),\ i \neq j,\ (i, j = 1,2, ..m)$$

We can now find an expression for the row sums of G, in terms of the $\{\alpha_k\}$ parameters of the g-inverse, the π_j and the m_{ij}.

If $\delta_j \equiv \sum_{k \neq j} \beta_k m_{kj}$ (j = 1,…, m) then

$$g_{i\bullet} = 1 + \gamma + \sum_{k \neq i} \pi_k \alpha_k m_{ik} - \sum_{k=1}^{m} \pi_k \alpha_k \delta_k .$$

By expressing g_{ij} in terms of h_{ij} we can find an expression for the elements of any g-inverse of $I - P$.

In particular, from $H = G(I - \Pi)$, $g_{ij} = h_{ij} + g_{i\bullet}\pi_j$.

This leads to the following KEY result

KEY THEOREM

Let $G = [g_{ij}] = G(\boldsymbol{\alpha}, \boldsymbol{\beta}, \gamma)$ be any g-inverse of $I - P$.

Then the g_{ij} can be expressed in terms of the parameters $\{\alpha_j\}$, $\{\beta_j\}$, γ, the stationary probabilities $\{\pi_j\}$, and the mean first passage times $\{m_{ij}\}$, of the Markov chain as

$$g_{ij} = \begin{cases} \left(1 + \gamma + \delta_j - m_{ij} + \sum_{k \neq i} \pi_k \alpha_k m_{ik} - \sum_{k=1}^{m} \pi_k \alpha_k \delta_k\right) \pi_j, & i \neq j, \\ \left(1 + \gamma + \delta_j + \sum_{k \neq j} \pi_k \alpha_k m_{jk} - \sum_{k=1}^{m} \pi_k \alpha_k \delta_k\right) \pi_j, & i = j. \end{cases}$$

where $\delta_j \equiv \sum_{k \neq j} \beta_k m_{kj}$ $(j = 1, \ldots, m)$.

New interconnections

For all $G = G(\boldsymbol{\alpha},\boldsymbol{\beta},\gamma)$ one condition g-inverses of $I - P$,

with $\delta_j = \sum_{k \neq j} \beta_k m_{kj}$,

$$g_{ij} = \begin{cases} \pi_j(\delta_j + g_{i\bullet} - m_{ij}), & i \neq j, \\ \pi_j(\delta_j + g_{j\bullet}), & i = j. \end{cases}$$

leading to the alternative expression

$$\delta_j = \frac{g_{jj}}{\pi_j} - g_{j\bullet}.$$

Special cases 1: $\delta_j \equiv \sum_{k \neq j} \beta_k m_{kj}$ (j = 1,…, m).

$$G = G(\mathbf{e}, \boldsymbol{\beta}, \gamma) \in A\{1,\ 5a\}$$

$$g_{ij} = \begin{cases} \pi_j(\delta_j + 1 + \gamma - m_{ij}), & i \neq j, \\ \pi_j(\delta_j + 1 + \gamma), & i = j. \end{cases}$$

$$G = G(\mathbf{e}, \boldsymbol{\beta}, -1) \in A\{1,\ 2,\ 5a\}$$

$$g_{ij} = \begin{cases} \pi_j(\delta_j - m_{ij}), & i \neq j, \\ \pi_j \delta_j, & i = j. \end{cases}$$

Special cases 2: $\eta_j \equiv \left(\sum_{k \neq j} m_{kj}\right) / m, \quad (j = 1, \ldots, m).$

$$G = G(\mathbf{e},\ \mathbf{e}/m, \gamma) \in A\{1,\ 4,\ 5a\}$$

$$g_{ij} = \begin{cases} \pi_j (1 + \gamma + \eta_j - m_{ij}), & i \neq j, \\ \pi_j (1 + \gamma + \eta_j), & i = j. \end{cases}$$

$G = G(\mathbf{e},\ \mathbf{e}/m, -1) \in A\{1,\ 2,\ 4,\ 5a\}$ (unique g-inverse)

$$g_{ij} = \begin{cases} \pi_j (\eta_j - m_{ij}), & i \neq j, \\ \pi_j \eta_j, & i = j. \end{cases}$$

Special cases 3: $\tau_j \equiv \sum_{k=1}^{m} \pi_k m_{kj} = \sum_{k \neq j} \pi_k m_{kj} + 1.$

$G = G(\mathbf{e}, \boldsymbol{\pi}, \gamma) \in A\{1,\ 5\}$

$$g_{ij} = \begin{cases} \pi_j(\tau_j + \gamma - m_{ij}), & i \neq j, \\ \pi_j(\tau_j + \gamma), & i = j. \end{cases}$$

$Z = G(\mathbf{e}, \boldsymbol{\pi}, 0) \in A\{1,\ 5\}$ with $\gamma = 0$ (unique, fundamental matrix)

$$g_{ij} = \begin{cases} \pi_j(\tau_j - m_{ij}), & i \neq j, \\ \pi_j \tau_j, & i = j. \end{cases}$$

$A^{\#} = G(\mathbf{e}, \boldsymbol{\pi}, -1) \in A\{1,\ 2,\ 5\}$ (unique, group inverse)

$$g_{ij} = \begin{cases} \pi_j(\tau_j - 1 - m_{ij}), & i \neq j, \\ \pi_j(\tau_j - 1), & i = j. \end{cases}$$ (Ben-Ari, Neumann (2012))

Note re τ_j

Since $\quad m_{jj}^{(2)} + m_{jj} = 2m_{jj} \sum_{i=1}^{m} \pi_i m_{ij},$

$$\tau_j = \sum_{i=1}^{m} \pi_i m_{ij} = \frac{m_{jj}^{(2)} + m_{jj}}{2m_{jj}} = \frac{1}{2} + \frac{m_{jj}^{(2)}}{2m_{jj}} = \frac{1 + \pi_j m_{jj}^{(2)}}{2}.$$

[In Hunter (2008) expressions for τ_j in terms of elements of g-inverses of $I - P$ are given.]

Special case 4:

$$G = G(\boldsymbol{\pi} / \boldsymbol{\pi}^T \boldsymbol{\pi}, \mathbf{e}/m, -1) \in A\{1,\ 2,\ 3,\ 4\} \text{ (Moore-Penrose)}$$

$$g_{ij} =$$

$$\begin{cases} \left(\eta_j - m_{ij} + (1 \big/ \sum \pi_k^2) \sum_{k \neq i} \pi_k^2 m_{ik} - (1 \big/ \sum \pi_k^2) \sum_{k=1}^{m} \pi_k^2 \eta_k \right) \pi_j, & i \neq j, \\ \left(\eta_j + (1 \big/ \sum \pi_k^2) \sum_{k \neq j} \pi_k^2 m_{ik} - (1 \big/ \sum \pi_k^2) \sum_{k=1}^{m} \pi_k^2 \eta_k \right) \pi_j, & i = j. \end{cases}$$

where $\eta_j \equiv \left(\sum_{k \neq j} m_{kj} \right) \big/ m, \quad (j = 1, \ldots, m).$

8. G-inverses in terms of stationary probs, first and second moments of passage times.

If $G = [g_{ij}] = G(\boldsymbol{e}, \boldsymbol{\pi}, \gamma) \in A\{1, 5\}$

$$g_{ij} = \begin{cases} \pi_j\left(\gamma + \dfrac{\pi_j m_{jj}^{(2)} + 1}{2} - m_{ij}\right), & i \neq j, \\ \pi_j\left(\gamma + \dfrac{\pi_j m_{jj}^{(2)} + 1}{2}\right), & i = j. \end{cases}$$

Special cases: Z = $G(\boldsymbol{e}, \boldsymbol{\pi}, 0)$ and $A^{\#} = G(\boldsymbol{e}, \boldsymbol{\pi}, -1)$.

Result for $A^{\#}$ given by Ben-Ari and Neumann (2012) - using analytic continuation, Laurent expansions and Taylor series expansions of generating functions.

9. Kemeny's constant.

$$K = \sum_{j=1}^{m} \pi_j m_{ij} = \sum_{j \neq i} \pi_j m_{ij} + 1.$$

The interesting observation is that this sum is in fact a constant, independent of *i*.

This is in contrast to $\tau_j = \sum_{i=1}^{m} \pi_i m_{ij} = \sum_{i \neq j} \pi_i m_{ij} + 1.$

which varies with j

If $G = [g_{ij}]$ is any generalised inverse of $I - P$,

$$K = 1 + \sum_{j=1}^{m} (g_{jj} - g_{j\bullet}\pi_j).$$

If $G = G(\boldsymbol{e}, \boldsymbol{\beta}, \gamma) \in$ A{1, 5a}, $K = tr(G) - \gamma.$

In particular, $K = tr(Z) = tr(A^{\#}) + 1.$

Simplification properties

For all $G = G(\alpha,\beta,\gamma)$, one condition g-inveres of $I - P$,

let $\delta_j = \sum_{k \neq j} \beta_k m_{kj}$.

Then $\qquad \sum_{k=1}^{m} \pi_k \delta_k = K - 1,$

where $K = \sum_{j=1}^{m} \pi_j m_{ij}$ is Kemeny's constant

(constant for all j = 1, 2, ..., m.)

References 1

Ben-Ari, I. & Neumann M. (2012). Probabilistic approach to Perron root, the group inverse, and applications, *Linear and Multilinear Algebra*, **60** (1), 39-63

Erdelyi, I. (1967). On the matrix equation $Ax = Bx$. *J. Math. Anal. Appl*. **17**, 119-132.

Hunter, J.J. (1969). On the moments of Markov renewal processes, *Adv. Appl. Probab*., **1**, 188 210.

Hunter, J.J. (1982). Generalized inverses and their application to applied probability problems, *Linear Algebra Appl*., **45**, 157-198.

Hunter, J.J. (1983). *Mathematical Techniques of Applied Probability, Volume 2, Discrete Time Models: Techniques and Applications*. Academic, New York.

Hunter J.J. (1986). 'Stationary distributions of perturbed Markov chains' *Linear Algebra Appl.* 82, 201-214.

Hunter, J.J. (1988). Characterisations of generalized inverses associated with Markovian kernels, *Linear Algebra Appl*., **102**, 121-142.

Hunter, J.J. (1990). Parametric forms for generalized inverses of Markovian kernels and their applications, *Linear Algebra Appl*., **127**, 71-84.

Hunter, J.J. (1992) "Stationary Distributions and Mean First Passage Times in Markov Chains using Generalized Inverses" *Asia-Pacific Journal of Operational Research*, **9**, 143-153, (1992)

Hunter, J. J. (2006). Mixing times with applications to perturbed Markov chains, *Linear Algebra Appl*., **417**, 108-123.

References 2

Hunter, J.J. (2007). “Simple procedures for finding mean first passage times in Markov chains” *Asia-Pacific Journal of Operational Research*, **34**, 813-829.

Hunter, J.J. (2008). Variances of First Passage Times in a Markov chain with applications to Mixing Times, *Linear Algebra Appl.,* **429**, 1135-1162.

Hunter, J.J. (2009) “Coupling and Mixing in a Markov chain” *Linear Algebra and it's Applications*, **430,** 2807 – 2821.

Kemeny, J.G. and Snell, J.L. (1960). *Finite Markov Chains*. Van Nostrand, New York.

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

Moore, E. H. (1920). On the Reciprocal of the General Algebraic Matrix. (Abstract), Bulletin of the American Mathematical Society **26**, 394-5.

Penrose, R. A. (1955). A Generalized Inverse for Matrices, *Proceedings of the Cambridge Philosophical Society* **51**, 406-13.

Paige, C.C., Styan, G.P.H., and Wachter, P.G. (1975). Computation of the stationary distribution of a Markov chain, *J. Statist. Comput. Simulation*, **4**, 173-186.