AUT COMPUTER + MATHEMATICAL SCIENCES

A comparison of computational techniques of the key properties of Markov Chains

> Jeffrey J Hunter Auckland University of Technology New Zealand



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1. Introduction

Let $P = [p_{ij}]$ be the transition matrix of an irreducible, discrete time Markov chain (MC) $\{X_n\}$ ($n \ge 0$). We are interested in developing accurate and efficient ways of finding the key properties of such MC's:

(*i*) the stationary probabilites $\{\pi_i\}$, $(1 \le j \le N)$

and hence the stationary probability vector $\boldsymbol{\pi}^{T}$ (*ii*) the mean first passage times $\{m_{ij}\}, (1 \le i, j \le N)$ and hence the mean first passage time matrix $M = [m_{ij}]$ (*iii*) the fundamental matrix of ergodic MC's, $Z = [I - P + \boldsymbol{e}\boldsymbol{\pi}^{T}]^{-1}$ (iv) the group inverse of the Markovian kernel, A = I - P, $A^{\#} = Z - \boldsymbol{e}\boldsymbol{\pi}^{T} = Z - \Pi$ 2. Stationary distributions of M.C.'s

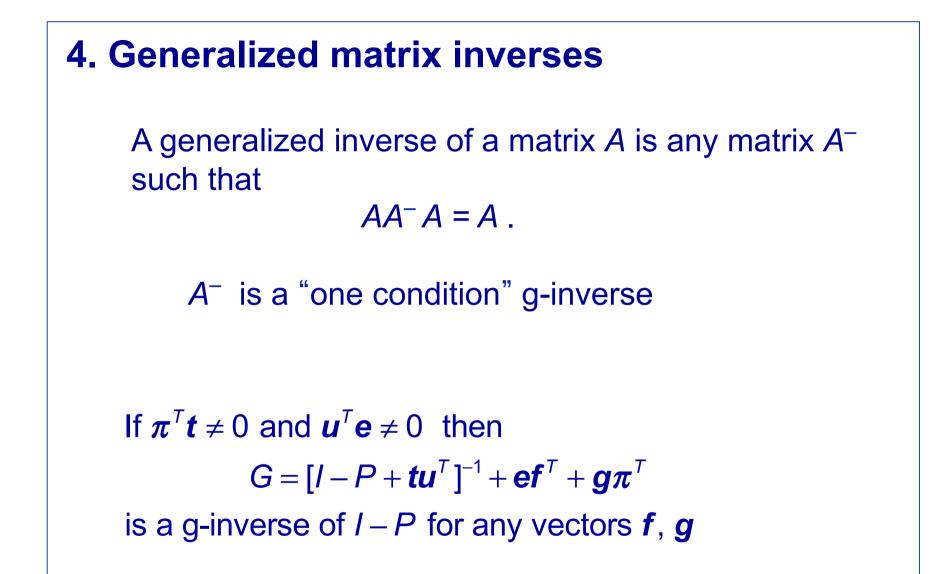
Let $\pi^T = (\pi_1, \pi_2, ..., \pi_N)$ be the stationary prob. vector of the Markov chain with transition matrix $P = [p_{ij}]$. Finite irreducible MC's $\{X_n\}$ have a unique stationary distribution $\{\pi_j\}, (1 \le j \le m)$, which for aperiodic (ergodic) M.C.s is the limiting distribution,

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

Further, the stationary probabilities $\{\pi_j\}$ satisfy the stationary equations

i.e.
$$\pi_{j} = \sum_{i=1}^{N} \pi_{i} p_{ij} \text{ with } \sum_{i=1}^{N} \pi_{i} = 1,$$
$$\pi^{T} (I - P) = \mathbf{0}^{T} \text{ with } \pi^{T} \mathbf{e} = 1.$$

3. Mean first passage times Let T_{ii} be the first passage time RV from state *i* to state *j*, i.e. T_{ii} = min { $n \ge 1$ such that $X_n = j$ given that $X_0 = i$ }. T_{ii} is the first return to state *i*. Let $m_{ii} = E[T_{ii} | X_0 = i]$, the mean first passage time from state *i* to state *j*. Let $M = [m_{ij}]$ be the matrix of mean first passage times It is well known that $m_{ij} = 1 + \sum p_{ik} m_{kj}$, with $m_{jj} = 1/\pi_j$. *M* satisfies the matrix equation (I-P)M = E - PD, where $E = [1] = ee^{T}$, and $D = M_d = [\delta_{ii}m_{ii}] = (\Pi_d)^{-1}$, $(\Pi = e\pi^{T})$.



5. The group inverse

Let *A* be a square matrix with real elements, such that $rank(A) = rank(A^2)$. The matrix $A^{\#}$ which satisfies

Condition 1: $AA^{\#}A = A$ Condition 2: $A^{\#}AA^{\#} = A^{\#}$ Condition 5: $AA^{\#} = A^{\#}A$

exists, is unique, and is called the "group inverse" of A.

i.e. A[#] is a 1-condition g-inverse with 2 additional conditions.

The group inverse of I - P has the form $A^{\#} = [I - P + \mathbf{e}\pi^{T}]^{-1} - \mathbf{e}\pi^{T} = [I - P + \Pi]^{-1} - \Pi$ (Meyer, 1975)



 $A^{\#}$ can be found from any g-inverse of I - P:

Let *G* is any g-inverse of I - P.

Let $K = (I - \Pi)G(I - \Pi)$

Then $K = A^{\#}$, the group inverse of I - P.

The group inverse from stationary probabilities and the mean first passage times

$$\begin{split} A^{\#} &= [a_{ij}^{\#}] \text{ can be found from the } m_{ij}: \\ a_{ij}^{\#} &= \begin{cases} \pi_j(\tau_j - 1), & i = j, \\ \pi_j(\tau_j - 1 - m_{ij}) = a_{jj}^{\#} - \pi_j m_{ij}, & i \neq j. \end{cases} \\ \text{where } \tau_j &\equiv \sum_{k=1}^N \pi_k m_{kj} = \sum_{k \neq j} \pi_k m_{kj} + 1. \\ \text{(Ben-Ari, Neumann, 2012),(Hunter, 2013).} \end{split}$$

6. Mean first passage times using g-inverses If G is any g-inverse of I - P, then $M = [G\Pi - E(G\Pi)_d + I - G + EG_d]D$. (Hunter, 1982)

(*i*) If Ge = ge then $M = [I - G + EG_d]D$.

(*ii*) Let G be any g-inverse of I - Pthen $H = G(I - \Pi)$ is a g-inverse of I - P with He = 0and $M = [I - H + EH_d]D$.

In particular, $M = [I - A^{\#} + EA_{d}^{\#}]D$, so that if $A^{\#} = [a_{ij}^{\#}]$,

 $m_{jj} = \frac{1}{\pi_j}$ and $m_{jj} = \frac{a_{jj}^{\#} - a_{jj}^{\#}}{\pi_j}, (i \neq j).$

7. Computational considerations

"The computation of *M* using $A^{\#}$ yields 3 sources of error:

- 1. The algorithm for computing π^{T} .
- 2. The computation of the inverse of $I P + \Pi$ (This matrix may have negative elements)
- 3. The matrix evaluation of *M*.
 (The matrix multiplying *D* may have negative elements)".
 Heyman & Reeves (1989)

"deriving means of first passage times from the group inverse *A*[#] leads to a significant inaccuracy on the more difficult problems." "it does not make sense to compute the group inverse unless the individual elements of those matrices are of interest." Heyman & O'Leary (1995)

8. Computational techniques

- 1. Limits of matrix powers for stationary probabilities.
- 2. Using g-inverses for stationary probs, mean first passage times and group inverse
- 3. GTH algorithm for stationary probs
- 4. Perturbation Techniques for stationary probs, mean first passage times and group inverse
- 5. Extend the GTH algorithm for mean first passage times

9. The stationary distribution using ginverses

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

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

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

In particular if $G = [I - P + eu^T]^{-1}$ then $\pi^T = u^T G$

10. Solving for stationary distribution using the GTH Algorithm

Let $P_N = \left[p_{ij} \right] = \left[p_{ij}^{(N)} \right]$ be the $N \times N$ transition matrix associated with a M.C. $\{X_k, k \ge 0\}$ with state space $S_N = \{1, 2, ..., N\}$, and transition probabilities $p_{ij}^{(N)} = P\{X_{k+1} = j | X_k = i\}.$

The general approach is to start with an *N*-state Markov chain and reduce the state space by one state at each stage. Thus in stages $S_N = S_{N-1} \cup \{N\}, \ S_{N-1} = S_{N-2} \cup \{N-1\}, ..., \ S_2 = \{1,2\}.$

From S_2 expand the state space one state at a time until we return to S_N

If M.C. is irreducible with state space S_N Let the stationary probability vector be $\boldsymbol{\pi}^T = (\pi_1, \pi_2, ..., \pi_{N-1}, \pi_N)$ $= \boldsymbol{\pi}^{(N)T} = (\pi_1^{(N)}, \pi_2^{(N)}, ..., \pi_{N-1}^{(N)}, \pi_N^{(N)}).$

From the stationary equations for S_N express $\pi_N^{(N)}$ in terms of $\pi_1^{(N)}, \dots, \pi_{N-1}^{(N)}$:

$$\pi_{N}^{(N)} = \frac{\sum_{i=1}^{N-1} \pi_{i}^{(N)} p_{iN}^{(N)}}{\sum_{j=1}^{N-1} p_{Nj}^{(N)}}$$

and eliminate $\pi_N^{(N)}$ from the stationary equations.

Let
$$P_N = \begin{bmatrix} Q_{N-1}^{(N)} & p_{N-1}^{(N)(c)} \\ p_{N-1}^{(N)(r)T} & p_{NN}^{(N)} \end{bmatrix}$$

Partition the stationary probability vector $\pi^{(N)T} = (v^{(N-1)T}, \pi_N^{(N)})$ where $v^{(N-1)T} = (\pi_1^{(N-1)}, \pi_2^{(N-1)}, ..., \pi_{N-1}^{(N-1)})$ It is easily shown that $v^{(N-1)T}(I_{N-1} - P_{N-1}) = \theta^T$, where $P_{N-1} = Q_{N-1}^{(N)} - \frac{p_{N-1}^{(N)(c)}p_{N-1}^{(N)(r)T}}{p_{N-1}^{(N)(r)T}e^{(N-1)}}$. Let $P_{N-1} = [p_{ij}^{(N-1)}]$ then $p_{ij}^{(N-1)} = p_{ij}^{(N)} + \frac{p_{iN}^{(N)}p_{Nj}^{(n)}}{S(N)}$, $1 \le i \le N-1$, $1 \le j \le N-1$

Note that calculation of the S(N) and the $p_{ij}^{(N-1)}$ do not involve subtractions.

Observe

$$\begin{split} P_{N-1} &\text{ is a stochastic matrix with state space } S_{N-1} \\ P_{N-1} &\text{ is irreducible} \\ \boldsymbol{v}^{(N-1)^{T}} &\text{ is a scaled stationary prob vector of this } N-1 \text{ state MC} \\ \boldsymbol{\pi}^{(N-1)^{T}} &= (\pi_{1}^{(N-1)}, \pi_{2}^{(N-1)}, \dots, \pi_{N-1}^{(N-1)}) \equiv \frac{1}{1-\pi_{N}^{(N)}} \boldsymbol{v}^{(N-1)^{T}} \\ &\text{ so that the first } N-1 \text{ stationary probs of the } N\text{-state MC are} \\ &\text{ scaled versions of the } N-1 \text{ state MC}. \end{split}$$

We can repeat this process reducing the state space from n to n-1 (n=N, N-1, ..., 2) with the resulting MC having a stationary distribution that is a scaled version of the first n-1 components of the stationary distribution of the MC with n states.

Thus if
$$P_n = \left[p_{ij}^{(n)} \right]$$
 with $P_{n-1} = \left[p_{ij}^{(n-1)} \right]$ then
 $p_{ij}^{(n-1)} = p_{ij}^{(n)} + \frac{p_{in}^{(n)} p_{nj}^{(n)}}{S(n)}, 1 \le i \le n-1, 1 \le j \le n-1;$

where $S(n) = 1 - p_{nn}^{(n)} = \sum_{j=1}^{n-1} p_{nj}^{(n)}$.

The $p_{ij}^{(n-1)}$ can be interpreted as the transition probability from *i* to *j* of the *M.C.* on S_n restricted to S_{n-1} . Since the original M.C. is irreducible (i.e. every state can be reached from every other state) the restricted M.C. must also be irreducible and further since $p_{nn}^{(n)} < 1$, S(n) > 0. If we start with

 $\boldsymbol{\pi}^{(N)T} = (\pi_1^{(N)}, \pi_2^{(N)}, \dots, \pi_{N-1}^{(N)}, \pi_N^{(N)}) \equiv (\pi_1, \pi_2, \dots, \pi_{n-1}, \pi_n)$ then the N-1 elements of $\boldsymbol{\pi}^{(N-1)T}$ are scaled elements of the first N-1 elements of $\boldsymbol{\pi}^{(N)T}$ and hence of $\pi_1, \pi_2, \dots, \pi_{n-1}$. Thus each $\boldsymbol{\pi}^{(n)T}$ is a scaled version of $(\pi_1, \pi_2, \dots, \pi_{n-1}, \pi_n)$.

The process continues to n = 2, where we have

 $P_{2} = \begin{bmatrix} p_{11}^{(2)} & p_{12}^{(2)} \\ p_{21}^{(2)} & p_{22}^{(2)} \end{bmatrix}$ which is a stochastic matrix.

The stationary distribution of this MC will be a scaled version of $\pi^{(2)T} = (\pi_1^{(2)}, \pi_2^{(2)})$ or of (π_1, π_2) .

The second stationary equation is $\pi_2 = \pi_1 p_{12}^{(2)} + \pi_2 p_{22}^{(2)}$ implying

$$\pi_2 = \pi_1 \frac{p_{12}^{(2)}}{S(2)}.$$

Note that $S(2) = 1 - p_{22}^{(2)} = \sum_{j=1}^{1} p_{2j}^{(2)} = p_{21}^{(2)} = p_{1}^{(2)(r)T} e^{(1)}$.

We now proceed with increasing the state space.

$$\pi_{3} = \frac{\sum_{i=1}^{2} \pi_{i} p_{i3}^{(3)}}{\sum_{i=1}^{2} p_{3i}^{(3)}} = \pi_{1} \frac{p_{13}^{(3)}}{S(3)} + \pi_{2} \frac{p_{23}^{(3)}}{S(3)},$$

In general, $\pi_{n} = \frac{\sum_{i=1}^{n-1} \pi_{i} p_{in}^{(n)}}{\sum_{i=1}^{n-1} p_{ni}^{(n)}} = \sum_{i=1}^{n-1} \pi_{i} \frac{p_{in}^{(n)}}{S(n)}$

GTH Algorithm

1. Start with a Markov chain with *N* states and transition matrix $P_N = [p_{ij}^{(N)}]$.

$$p_{ij}^{(n-1)} = p_{ij}^{(n)} + \frac{p_{in}^{(n)} p_{nj}^{(n)}}{S(n)}, 1 \le i \le n - 1, 1 \le j \le n - 1; \text{ where}$$

$$S(n) = \sum_{j=1}^{n-1} p_{nj}^{(n)}.$$
3. Set $r_1 = 1$ and compute $r_n = \frac{\sum_{i=1}^{n-1} r_i p_{in}^{(n)}}{S(n)}, \text{ for } n = 2,...,N.$
4. Compute $\pi_i = \frac{r_i}{\sum_{j=1}^{N} r_j}, i = 1, 2, ..., N.$

11. Solving for stationary distributions, mean first passage times and group inverse using perturbation procedures

The basic ideas are very simple: Start with a transition matrix P_{α} with known stat prob vector π_0^T , mean first passage time matrix M_{0} , and group inverse $A_{0}^{\#}$ for $I - P_{0}$, (or g-inverse G_{0}). Sequentially change P_0 by replacing the *i*th row of P_0 with the i^{th} row, \boldsymbol{p}_i^T , of P (i = 1, 2, ..., N) to obtain P_i with $P_{N} = P$. Thus, if $P_0 = \sum_{i=1}^{N} \mathbf{e}_i \mathbf{p}_{(0)i}^T$, and $P = \sum_{i=1}^{N} \mathbf{e}_i \mathbf{p}_i^T$ then $P_i = P_{i-1} + \mathbf{e}_i \mathbf{b}_i^T$ with $\boldsymbol{b}_{i}^{T} = \boldsymbol{p}_{i}^{T} - \boldsymbol{p}_{(0)i}^{T}$ for i = 1, 2, ..., N. Update π_{i-1}^T , M_{i-1} and $A_{i-1}^\#$ (or G_{i-1}) to π_i^T , M_i and $A_i^\#$ (or G_i) stopping with $\pi_{N}^{T} = \pi^{T}, M_{N} = M$ and $A_{N}^{\#} = A^{\#}$ (or $G_{N} = G$).

Choice of P₀

We require P_0 to be irreducible. The simplest structure is

$$P_{0} = \begin{bmatrix} 1/m & 1/m & \dots & 1/m & \dots & 1/m \\ 1/m & 1/m & \dots & 1/m & \dots & 1/m \\ \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 1/m & 1/m & \dots & 1/m & \dots & 1/m \\ \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 1/m & 1/m & \dots & 1/m & \dots & 1/m \end{bmatrix} = \frac{1}{m} \mathbf{e} \mathbf{e}^{\mathsf{T}} = \frac{1}{m} \mathsf{E}$$

This leads to

$$M_{0} = m\mathbf{e}\mathbf{e}^{T} = mE$$

$$A_{0}^{\#} = I - \frac{1}{m}\mathbf{e}\mathbf{e}^{T} = I - \frac{1}{m}E$$

and

The perturbation algorithms

We consider six techniques

- 1. Extend the procedure of Hunter (JAMSA, 1991) using a family of 1-condition generalized inverse updates to find successive stat prob vectors with extensions to the group inverses.
- 2. Consider successive direct row perturbation updates of the group inverse (and hence the mean first passage times).
- 3. Consider a blend of 1. and 2. through updating using matrix procedures for the stat probability vectors and the group inverses in tandem.

12. The algorithms

Procedure based on updating specific ginverses of I - P of the form $G = [I - P + e\beta^T]^{-1}$ have simple forms for the MFPT matrix since

Ge = ge. 4. $\boldsymbol{\beta}^{T} = \frac{\mathbf{e}^{T}}{N}$, with $G = G_{e} \equiv \left[I - P + \frac{\mathbf{e}\mathbf{e}^{T}}{N}\right]^{-1}$. 5. $\beta^{T} = \mathbf{e}_{1}^{T}$, with $G = G_{e_{1}} = [I - P + \mathbf{e}\mathbf{e}_{1}^{T}]^{-1}$ 6. $\beta^{T} = \mathbf{e}^{T}$, with $G = G_{ee} = [I - P + \mathbf{e}\mathbf{e}^{T}]^{-1}$ Note that it is easy to find the group inverse from the MFPT matrix since in these cases $A^{\#} = (I - \mathbf{e}\boldsymbol{\pi}^{T})G.$

Perturbation procedures for stat distribns

With
$$P_0 = \mathbf{e}\mathbf{e}^T/m$$
,
 $P_i = P_{i-1} + \mathbf{e}_i \mathbf{b}_i^T$ with $\mathbf{b}_i^T = \mathbf{p}_i^T - \mathbf{e}^T/m$.
With $\mathbf{t}_0 = \mathbf{e}$ and $\mathbf{u}_0^T = \mathbf{e}^T/m$
then $G_0 = [I - P_0 + \mathbf{t}_0 \mathbf{u}_0^T]^{-1} = I$ and $\pi_0^T = \frac{\mathbf{u}_0^T G_0}{\mathbf{u}_0^T G_0 \mathbf{e}} = \mathbf{e}^T/m$.
Let $\mathbf{t}_i = \mathbf{e}_i$ and $\mathbf{u}_i^T = \mathbf{u}_{i-1}^T + \mathbf{b}_i^T = \mathbf{u}_{i-1}^T + \mathbf{p}_i^T - \mathbf{e}^T/m$,
then $G_i = [I - P_i + \mathbf{t}_i \mathbf{u}_i]^{-1} = G_{i-1}[I + (\mathbf{e}_{i-1} - \mathbf{e}_i)(\pi_{i-1}^T/\pi_{i-1}^T \mathbf{e}_i)]$
implying $\pi_i^T = \frac{\mathbf{u}_i^T G_i}{\mathbf{u}_i^T G_i \mathbf{e}}$, $i = 1, 2, ..., m$.

(*i*) Let
$$G_0 = I$$
, $u_0^T = e^T/N$.
(*ii*) For $i = 1, 2, ..., N$, let $p_i^T = e_i^T P$,
 $u_i^T = u_{i-1}^T + p_i^T - e^T/N$,
 $G_i = G_{i-1} + G_{i-1}(e_{i-1} - e_i)(u_{i-1}^T G_{i-1}/u_{i-1}^T G_{i-1}e_i)$.
(*iii*) At $i = N$, let $G = G_N$ and
 $\pi^T = \pi_N^T = \frac{u_N^T G_N}{u_N^T G_N e}$.
(*iv*) Compute $H = G(I - e\pi^T)$.
(*v*) Compute $A^\# = (I - e\pi^T)H$.
(*vi*) Compute $M = [I - H + EH_d]D$ where $D = ((e\pi^T)_d)^{-1}$.

Perturbations of the Group Inverse

Let P = P + E where the perturbing matrix E has the property E e = 0. Let $\Pi = e\pi^T$ where π^T is the stat prob vector of the MC associated with *P*.

Let $A^{\#}$ and $\overline{A}^{\#}$ be the group inverses of A = I - P and $\overline{A} = I - \overline{P}$.

(*i*) $I - EA^{\#}$ is non-singular, (*ii*) the stat prob vector of the perturbed MC is $\overline{\pi}^{T} = \pi^{T} (I - EA^{\#})^{-1}$ (*iii*) the group inverse of $\overline{A} = I - \overline{P}$ is $\overline{A}^{\#} = A^{\#} (I - EA^{\#})^{-1} - \Pi (I - EA^{\#})^{-1} A^{\#} (I - EA^{\#})^{-1}$.

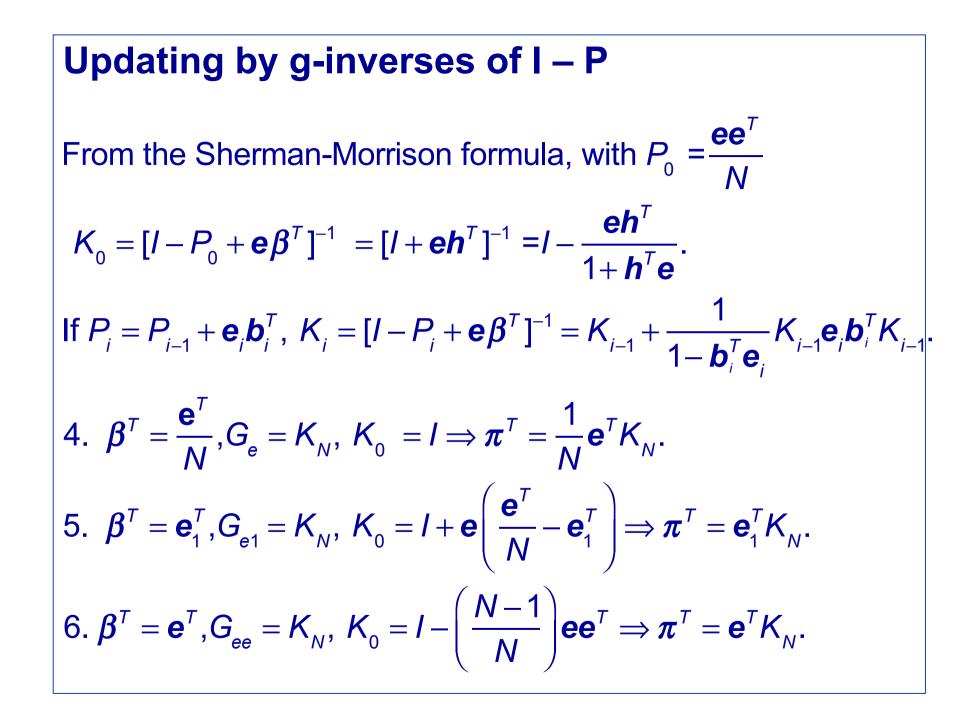
Row perturbations of the Group Inverse
Let
$$E = \mathbf{e}_i \mathbf{b}^T$$
, i.e. a perturbation to the *i*-th row with $\mathbf{b}^T \mathbf{e} \neq 0$,
 $\overline{\mathbf{\pi}}^T = \mathbf{\pi}^T \left[I + \frac{1}{1 - \mathbf{b}^T A^* \mathbf{e}_i} \mathbf{e}_i \mathbf{b}^T A^* \right]$ and
 $\overline{A}^* = A^* + \frac{1}{1 - \mathbf{b}^T A^* \mathbf{e}_i} A^* \mathbf{e}_i \mathbf{b}^T A^* - \mathbf{e} \mathbf{y}^T$,
where $\mathbf{y}^T = \left(\frac{\pi_i}{1 - \mathbf{b}^T A^* \mathbf{e}_i} \right) \mathbf{b}^T \left(A^* + \frac{\mathbf{b}^T (A^*)^2 \mathbf{e}_i}{1 - \mathbf{b}^T A^* \mathbf{e}_i} I \right) A^*$.
(Note that $\mathbf{y}^T \mathbf{e} = 0$.) See (Kirkland and Neumann, 2013).
Carry out row by row perturbations, with \mathbf{b}_i^T the change at
the *i*-th row, and A_i^* the group inverse after the *i*-th change.
 $A_i^* = R_i + \mathbf{e} \mathbf{y}_i^T \implies R_i = R_{i-1} + \frac{1}{1 - \mathbf{b}_i^T R_{i-1} \mathbf{e}_i} R_{i-1} \mathbf{e}_i \mathbf{b}_i^T R_{i-1}$ with $\mathbf{y}_i^T \mathbf{e} = 0$.

(i) Let
$$P_0 = \mathbf{e} \mathbf{e}^T / N \Rightarrow A_0^* = I - \mathbf{e} \mathbf{e}^T / N$$
. Take $R_0 = I - \mathbf{e} \mathbf{e}^T / N$.
(ii) For $i = 1, 2, ..., N$, let $\mathbf{p}_i^T = \mathbf{e}_i^T P$,
 $\mathbf{b}_i^T = \mathbf{p}_i^T - \mathbf{e}^T / N$,
 $R_i = R_{i-1} + \frac{1}{1 - \mathbf{b}_i^T R_{i-1} \mathbf{e}_i} R_{i-1} \mathbf{e}_i \mathbf{b}_i^T R_{i-1}$.
(iii) At $i = N$, let $R = R_N$ so that $A^* = R + \mathbf{e} \mathbf{y}_N^T$.
 $(I - P)A^* = I - \mathbf{e} \pi^T$ yields the stat prob vector:
 $\Rightarrow \pi^T = \mathbf{e}_1^T - \mathbf{e}_1^T (I - P) R$.
(iv) $\pi^T A^* = \mathbf{0}^T$ yields the group inverse:
 $\Rightarrow \mathbf{y}_N^T = -\pi^T R \Rightarrow A^* = (I - \mathbf{e} \pi^T) R$.
(v) Compute $M = [I - A^* + EA_d^*]D$ where $D = ((\mathbf{e} \pi^T)_d)^{-1}$.

Updating by matrix operations

Let P = P + E where E has the property Ee = 0. Let $\Pi = \mathbf{e} \pi^{T}$ and $\overline{\Pi} = \mathbf{e} \overline{\pi}^{T}$ where π^{T} and $\overline{\pi}^{T}$ are the stat prob vectors associated with P and P. $\overline{\pi}^{T} = \pi^{T} (I - \mathbf{E} \mathbf{A}^{\#})^{-1} \Longrightarrow \overline{\Pi} = \Pi (I - \mathbf{E} \mathbf{A}^{\#})^{-1}.$ Under the perturbation $E = \mathbf{e}_i \mathbf{b}^T$ to the *i*-th row with $\mathbf{b}^T \mathbf{e} \neq 0$, $(I - EA^{\#})^{-1} = I + \frac{1}{1 - \boldsymbol{b}^{T} A^{\#} \boldsymbol{e}_{i}} \boldsymbol{e}_{i} \boldsymbol{b}^{T} A^{\#}$ so that $\overline{\Pi} = \Pi \left| I + \frac{1}{1 - \boldsymbol{b}^T A^{\#} \boldsymbol{e}_{\perp}} \boldsymbol{e}_{i} \boldsymbol{b}^T A^{\#} \right| \text{ and }$ $\overline{A}^{\#} = (I - \overline{\Pi})A^{\#}(I - EA^{\#})^{-1} = (I - \overline{\Pi})A^{\#}\left(I + \frac{1}{1 - \boldsymbol{b}^{T}A^{\#}\boldsymbol{e}_{i}}\boldsymbol{e}_{i}\boldsymbol{b}^{T}A^{\#}\right).$

(i) Let
$$P_0 = \mathbf{e} \mathbf{e}^T / N \Rightarrow \Pi_0 = \mathbf{e} \mathbf{e}^T / N$$
, $A_0^{\#} = I - \mathbf{e} \mathbf{e}^T / N$.
(ii) For $i = 1, 2, ..., N$, let $\mathbf{p}_i^T = \mathbf{e}_i^T P$, $\mathbf{b}_i^T = \mathbf{p}_i^T - \mathbf{e}^T / N$,
 $\mathbf{S}_i = I + \frac{1}{1 - \mathbf{b}_i^T A_{i-1}^{\#} \mathbf{e}_i} \mathbf{e}_i \mathbf{b}_i^T A_{i-1}^{\#}$,
 $\Pi_i = \Pi_{i-1} \mathbf{S}_i$,
 $A_i^{\#} = (I - \Pi_i) A_{i-1}^{\#} \mathbf{S}_i$.
(iii) At $i = N$, let $\mathbf{S} = \mathbf{S}_N$ then
 $\Pi = \Pi_{N-1} \mathbf{S}$,
 $A^{\#} = (I - \Pi_i) A_{N-1}^{\#} \mathbf{S}$.
(iv) Compute $M = [I - A^{\#} + E A_d^{\#}] D$, where $D = (\Pi_d)^{-1}$.



(*i*) Let
$$K_0 = I$$
.
(*ii*) For $i = 1, 2, ..., N$, let $p_i^T = e_i^T P, b_i^T = p_i^T - e^T / N$.
 $K_i = K_{i-1}(I + C_i)$ where $k_i = 1 - e_i K_{i-1} e_i$ and $C_i = \frac{1}{k_i} e_i b_i^T K_{i-1}$
(*iii*) At $i = N$, let $K = K_N$ then $\pi^T = \frac{1}{N} e^T K$.
(*v*) Compute $A^{\#} = (I - e\pi^T) K$.
(*vi*) Compute $M = [I - K + EK_d] D$ where $D = ((e\pi^T)_d)^{-1}$.

(i) Let
$$K_0 = I + \mathbf{e} \left(\frac{\mathbf{e}^T}{N} - \mathbf{e}_1^T \right)$$

(ii) For $i = 1, 2, ..., N$, let $\mathbf{p}_i^T = \mathbf{e}_i^T P, \mathbf{b}_i^T = \mathbf{p}_i^T - \mathbf{e}^T / N$.
 $K_i = K_{i-1}(I + C_i)$ where $k_i = 1 - \mathbf{e}_i K_{i-1} \mathbf{e}_i$ and $C_i = \frac{1}{k_i} \mathbf{e}_i \mathbf{b}_i^T K_{i-1}$
(iii) At $i = N$, let $K = K_N$ then $\pi^T = \mathbf{e}_1^T K$.
(v) Compute $A^\# = (I - \mathbf{e}\pi^T)K$.
(vi) Compute $M = [I - K + EK_d]D$ where $D = ((\mathbf{e}\pi^T)_d)^{-1}$.

(i) Let
$$K_0 = I - \left(\frac{N-1}{N}\right) \mathbf{e} \mathbf{e}^T$$
.
(ii) For $i = 1, 2, ..., N$, let $\mathbf{p}_i^T = \mathbf{e}_i^T P, \mathbf{b}_i^T = \mathbf{p}_i^T - \mathbf{e}^T / N$.
 $K_i = K_{i-1}(I+C_i)$ where $k_i = 1 - \mathbf{e}_i K_{i-1} \mathbf{e}_i$ and $C_i = \frac{1}{k_i} \mathbf{e}_i \mathbf{b}_i^T K_{i-1}$
(iii) At $i = N$, let $K = K_N$ then $\pi^T = \mathbf{e}^T K$.
(v) Compute $A^\# = (I - \mathbf{e}\pi^T)K$.
(vi) Compute $M = [I - K + EK_d]D$ where $D = ((\mathbf{e}\pi^T)_d)^{-1}$.

12. Standard procedures – MFPT's

The "standard algorithm" is $M = [I - Z + EZ_d]D$ where $Z = [I - P + e\pi^T]^{-1}$, Kemeny and Snell's "fundamental matrix"

Simple procedure for MFPTs

Hunter (2007) presented a "**simple algorithm**" which is the simplest method to simultaneoulsy compute the stationary distribution and the MFPTs.

If
$$G_{eb} = [I - P + ee_b^T]^{-1} = |g_{ij}|,$$

then
$$\pi_{j} = g_{bj}, \quad j = 1, 2, ..., N,$$

and $m_{ij} = \begin{cases} 1/g_{bj}, & i = j, \\ (g_{jj} - g_{ij})/g_{bj}, & i \neq j. \end{cases}$

13. Mean First Passage Times via Extended GTH

We seek a computational procedure, utilising the GTH/State reduction procedure.

For a M.C. { X_n } with *N*-states and transition matrix *P*, its mean first passage time matrix (MFPT) *M* satisfies $(I-P)M = E - PM_d$ where $E = [1] = e^{(N)}e^{(N)T}$ and $M_d = [\delta_{ij}m_{jj}] = diag(\pi_1, \pi_2, ..., \pi_N).$

For a M.R.P. { X_n , T_n } the MFPT matrix satisfies $(I - P)M = \mu^{(N)}e^{(N)T} - P(M)_{d}$

 $F_{ii}(t)$ is the distribution function of the "holding time" $T_{n+1} - T_n$ in state X_n until transition into state X_{n+1} given that the M.R.P. makes a transition from X_n to X_{n+1} . Let $\mu_{ij} = \int_{0}^{\infty} t \, dQ_{ij}(t)$ so that $\mu_{ij} = \rho_{ij} E[T_{n+1} - T_n | X_n = i, X_{n+1} = j].$ Let $P^{(1)} = \left[\mu_{ii} \right]$ then $(I-P)M = P^{(1)}E - PM_{a}$ Let $\mu = P^{(1)}e$ then $\mu^T = (\mu_1, \mu_2, ..., \mu_N)$ where $\mu_i = \sum_{i=1}^N \mu_{ii}$. $\mu_i = E[T_{n+1} - T_n | X_n = i]$ is the "mean holding time in state *i*". Thus $P^{(1)}E = P^{(1)}ee^{T} = \mu e^{T}$

Note that for a M.C. $\mu^{(N)T} = e^{(N)T} = (1, 1, ..., 1)$ and $P^{(1)}E = E$

Let us partition
$$M = M_N$$
 as $M_N = \begin{bmatrix} M_{N-1} & m_{N-1}^{(N)(c)} \\ m_{N-1}^{(N)(r)T} & m_{NN} \end{bmatrix}$
where
 $M_{N-1} = \begin{bmatrix} m_{ij} \end{bmatrix}$, $(1 \le i \le N - 1, 1 \le j \le N - 1)$,
 $m_{N-1}^{(N)(r)T} = (m_{N1}, m_{N2}, ..., m_{N,N-1})$ and
 $m_{N-1}^{(N)(c)T} = (m_{1N}, m_{2N}, ..., m_{N-1,N}).$

Let us also partition $\mu^{(N)T} = (\mu_1^{(N)}, \dots, \mu_{N-1}^{(N)}, \mu_N^{(N)}) = (\mu_{N-1}^{(N)T}, \mu_N^{(N)})$ where $\mu_{N-1}^{(N)T} = (\mu_1^{(N)}, \dots, \mu_{N-1}^{(N)})$

Expressing $(I - P)M = \mu^{(N)}e^{(N)T} - P(M)_d$ in block form and carrying out block multiplication we obtain the following results (details omitted). Using the expression for P_{N-1} , as derived for the GTH algorithm, it is easily seen that

$$(I_{N-1} - P_{N-1})M_{N-1} = \mu^{(N-1)}e^{(N-1)T} - P_{N-1}(M_{N-1})_{d},$$

where $\mu^{(N-1)} = \mu_{N-1}^{(N)} + \frac{\mu_{N}^{(N)}p_{N-1}^{(N)(c)}}{p_{N-1}^{(N)(r)T}e^{(N-1)}}.$
Further, $m_{N-1}^{(N)(r)T} = \frac{\left\{ p_{N-1}^{(N)(r)T} \left(M_{N-1} - (M_{N-1})_{d} \right) + \mu_{N}^{(N)}e^{(N-1)T} \right\}}{p_{N-1}^{(N)(r)T}e^{(N-1)}}$
implying $m_{Nj} = \frac{\left\{ \sum_{k=1,k\neq j}^{N-1} p_{Nk}^{(N)}m_{kj} + \mu_{N}^{(N)} \right\}}{S(N)}$ for $1 \le j \le N-1$,

leading to expressions for m_{Nj} in terms of $m_{1j},...,m_{kj},...,m_{N-1,j}$ $(k \neq j)$, i.e. expressions for m_{Nj} in terms of the remaining elements of the j – th column of M.

More difficult to find $m_{N-1}^{(N)(c)}$, i.e. the m_{iN} for $1 \le i \le N-1$. $(I_{n-1} - Q_{n-1}^{(n)})m_{n-1}^{(n)(c)} = \mu_{n-1}^{(n)}$ $\left|Q_{N-1}^{(N)} = \left\lceil p_{ii}^{(N)} \right\rceil$ for $1 \le i \le N-1$, $1 \le j \le N-1$, an $(n-1) \times (n-1)$ matrix derived from P_N , requires further step by step reduction procedure by eliminating m_{N-1N} from $m_{N-1}^{(N)(c)T}$ replacing it in the expressions for the elements $m_{1N}, m_{2N}, \dots, m_{N-2N}$. Need to express $(N-1) \times (N-1)$ matrix $Q_{N-1}^{(N)}$ in block form. $m_{N-1,N} = \frac{\left\{ p_{N-2}^{(N-1)(N)(r)T} m_{N-2}^{(N)(c)} + \mu_{N-1}^{(N)} \right\}}{1 - p_{N-1,N-1}^{(N-1)}} = \frac{\left\{ \sum_{k=1}^{N-2} q_{N-1,k}^{(N-1)} m_{kN} + \mu_{N-1}^{(N)} \right\}}{R(N)},$ where $R(N) = 1 - p_{N-1,N-1}^{(N-1)} = \sum_{j=1, j \neq N-1}^{N} p_{N-1,j}^{(N)}$ (i.e. obtained from P_N).

Thus for a general reduction from *n* states to *n*-1 states

If
$$(I_n - P_n)M_n = \mu^{(n)}e^{(n)T} - P_n(M_n)_d$$
 where $\mu^{(n)T} = (\mu_{n-1}^{(n)}, \mu_n^{(n)})$,
then $(I_{n-1} - P_{n-1})M_{n-1} = \mu^{(n-1)}e^{(n-1)T} - P_{n-1}(M_{n-1})_d$
where $\mu^{(n-1)T} = \mu_{n-1}^{(n)T} + \frac{\mu_n^{(n)}p_{n-1}^{(n)(c)T}}{p_{n-1}^{(n)(c)T}e^{(n-1)}}$.
 $\mu^{(n)T} = (\mu_{n-1}^{(n)T}, \mu_n^{(n)})$ is a 1× *n* vector, $\mu_{n-1}^{(n)T} = (\mu_1^{(n)}, \dots, \mu_{n-1}^{(n)})$ and
 $\mu^{(n-1)T} = (\mu_1^{(n-1)}, \dots, \mu_{n-1}^{(n-1)})$ is a1× (*n*-1) vector, with
 $\mu_i^{(n-1)} = \mu_i^{(n)} + \frac{\mu_n^{(n)}p_{i,n}^{(n)}}{S(n)}$, $(1 \le i \le n-1)$.
where $S(n) = p_{n-1}^{(n)(r)T}e^{(n-1)} = \sum_{j=1}^{n-1}p_{jj}^{(n)} = 1 - p_{nn}^{(n)}$.

We can reduce the state space by 1 at successive steps retaining the same mean first passage times for the reduced state space i.e. $M_{n-1} = [m_{ij}]$, for $1 \le i \le n-1$, $1 \le j \le n-1$, although the calculation is modified with mean holding times in the states being modified. i.e. in effect we are using a MRP variant to preserve the mean first passage times for the reduced state space.

If we are given $M_{n-1} = [m_{ij}]$, $(1 \le i \le n-1, 1 \le j \le n-1)$, we wish to find $m_{n-1}^{(n)(c)}, m_{n-1}^{(n)(r)T}$ and m_{nn} .

First $m_{nn} = 1/\pi_n^{(N)}$ so we can use the GTH algorithm from the calculation of the stationary probabilities.

For
$$m_{n-1}^{(n)(c)}$$
, $m_{nj} = \frac{\left\{\sum_{k=1,k\neq j}^{n-1} p_{nk}^{(n)} m_{kj} + \mu_n^{(n)}\right\}}{S(n)}$ for $1 \le j \le n-1$.

For
$$n = 2$$
:
 $\begin{pmatrix} l_2 - P_2 \end{pmatrix} M_2 = \mu^{(2)} e^{(2)T} - P_2 (M_2)_d \\ \begin{bmatrix} 1 - p_{11}^{(2)} & -p_{12}^{(2)} \\ -p_{21}^{(2)} & 1 - p_{22}^{(2)} \end{bmatrix} \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \\ = \begin{bmatrix} \mu_1^{(2)} & \mu_1^{(2)} \\ \mu_2^{(2)} & \mu_2^{(2)} \end{bmatrix} - \begin{bmatrix} p_{11}^{(2)} m_{11} & p_{12}^{(2)} m_{22} \\ p_{21}^{(2)} m_{11} & p_{22}^{(2)} m_{22} \end{bmatrix} \\ \text{leading to} \\ M_2 = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} = \begin{bmatrix} \frac{p_{21}^{(2)} \mu_1^{(2)} + p_{12}^{(2)} \mu_2^{(2)}}{p_{21}^{(2)}} & \frac{\mu_1^{(2)}}{p_{12}^{(2)}} \\ \frac{\mu_2^{(2)}}{p_{21}^{(2)}} & \frac{p_{21}^{(2)} \mu_1^{(2)} + p_{12}^{(2)} \mu_2^{(2)}}{p_{12}^{(2)}} \end{bmatrix}$

General procedure for finding all the elements of *M*.

Step 1: .Start with P_N and concentrate on finding only the expressions for m_{i1} for i = 1, 2, ..., N. i.e. if $P_N = \left[p_{ij}^{(N)} \right]$ carry out the extended GTH algorithm For n = N, N-1, ..., 3,

let
$$p_{ij}^{(n-1)} = p_{ij}^{(n)} + \frac{p_{in}^{(n)}p_{nj}^{(n)}}{S(n)}$$
, $1 \le i \le n-1$, $1 \le j \le n-1$
and $\mu_i^{(n-1)} = \mu_i^{(n)} + \frac{\mu_n^{(n)}p_{i,n}^{(n)}}{S(n)}$, $(1 \le i \le n-1)$, with $S(n) = \sum_{j=1}^{n-1} p_{nj}^{(n)}$.
with $(\mu_1^{(N)}, \mu_2^{(N)}, \dots, \mu_N^{(N)}) = (1, 1, \dots, 1)$.

Let
$$m_{11} = \mu_1^{(2)} + \frac{\mu_{12}^{(2)} \mu_2^{(2)}}{p_{21}^{(2)}}$$
,
 $m_{21} = \frac{\mu_2^{(2)}}{S(2)}$,
 $m_{31} = -\frac{\frac{p_{32}^{(3)} m_{21} + \mu_3^{(3)}}{S(3)}}{S(3)}$,
 $m_{n1} = -\frac{\sum_{k=2}^{n-1} p_{nk}^{(n)} m_{k1} + \mu_n^{(n)}}{S(n)}$, $n = 3,...,N$.
This provides the entries of the first column of
 $M = [m_{ij}]$, i.e. $m_N^{(1)(N)}$, where
 $M = (m_N^{(1)(N)}, m_N^{(2)(N)}, ..., m_N^{(N)(N)})$ with $m_N^{(1)(N)T} = (m_{11}, m_{21}, ..., m_{N1})$

	1				
m ₁₁	m ₁₂	m ₁₃	m ₁₄	m ₁₅	
m ₂₁	m ₂₂	m ₂₃	m ₂₄	m ₂₅	
m ₃₁	m ₃₂	m ₃₃	m ₃₄	m ₃₅	
m ₄₁	m ₄₂	m ₄₃	m ₄₄	m ₄₅	
m ₅₁	m ₅₂	m ₅₃	m ₅₄	m ₅₅	

Step 2: Now reorder the rows of $P^{(N)}$ by moving the first column after the *N*th column, followed by moving the first row to the last row.

$P_N \equiv P_N^{(1)} =$	p ₁₁	p ₁₂		р _{1,N-1}	p _{1,N}	
	p ₂₁	p ₂₂		р _{2,N-1}	$p_{_{2N}}$	
$P_N \equiv P_N^{(1)} =$						
	$p_{_{N-1.1}}$	р _{N-1,2}		$p_{N-1,N-1}$	$p_{_{N-1,N}}$	
	р _{N1}	р _{N2}		$p_{_{N,N-1}}$	$p_{_{NN}}$	
	p_{22} $p_{N-1,2}$ p_{N2} p_{12}		р _{2,N-1}	p _{2N}	p ₂₁]
\rightarrow	<i>p</i> _{N-1,2}	ŀ	D _{N-1,N-1}	р _{N-1,N}	р _{N-1,1}	$\equiv P_N^{(2)}$
	р _{N2}		$p_{_{N,N-1}}$	$p_{_{NN}}$	p _{N.1}	
	<i>p</i> ₁₂		р _{1,N-1}	$p_{_{1,N}}$	p ₁₁	

Step 3: Carry out the algorithm, as in Step 1, with $P_{\Lambda} = P_{\Lambda}^{(2)}$ to obtain the vector of MFPTs which we label as $\overline{m_N}^{-(2)(N)}$ where $\overline{m}_{N}^{(2)(N)T} = (m_{22}, m_{32}, \dots, m_{N2}, m_{12}).$ Step 4: Reorder $P_2^{(N)}$ as in step 2 to obtain $P_3^{(N)}$ and repeat Step 3 to obtain $\overline{m}^{(3)(N)}$ where $\overline{m}^{(3)(N)T} = (m_{33}, m_{43}, \dots, m_{N3}, m_{13}, m_{23})$ Step k: Repeat as above with $P_{k}^{(N)}$ to obtain $\overline{m}^{(k)(N)}$ where $\overline{m}^{(k)(N)T} = (m_{kk}, m_{k+1,k}, \dots, m_{N,k}, m_{1,k}, \dots, m_{k-1,k})$ finishing with $P_{N}^{(N)}$ and $\overline{m}^{(N)(N)}$ where $\overline{m}^{(N)(N)T} = (m_{NN}, m_{1,N}, m_{2,N}, ..., m_{N-1,N})$ Step *N* + 1: Let $\overline{M} = (m_N^{(1)(N)}, \overline{m}_N^{(2)(N)}, \dots, \overline{m}_N^{(N)(N)})$ Finally reorder *M* to obtain $M = (m_N^{(1)(N)}, m_N^{(2)(N)}, \dots, m_N^{(N)(N)})$

14. Test Problems

Introduced by Harrod & Plemmons (1984) and considered by others in different contexts.

TP1: The original transition matrix was not irreducible and was replaced (Heyman (1987), Heyman & Reeves (1989)) by

TP2 (Also Benzi (2004))

-								٦
.85	0	.149	.0009	0	.00005	0	.00005	
.1	.65	.249	0	.00009	.00005	0	.00005	
.1	.8	.09996	.0003	0	0	.0001	0	
0	.0004	0	.7	.2995	0	.0001	0	
.0005	0	.0004	.399	.6	.0001	0	0	ľ
0	.00005	0	0	.00005	.6	.2499	.15	
.00003	0	.00003	.00004	0	.1	.8	.0999	
0	.00005	0	0	.00005	.1999	.25	.55	
	.1 .1 0 .0005 0	.1.65.1.80.0004.000500.00005.000030	.1.65.249.1.8.099960.00040.00050.00040.000050.000030.00003	.1.65.2490.1.8.09996.00030.00040.7.00050.0004.3990.0000500.000030.00003.00004	.1.65.2490.00009.1.8.09996.000300.00040.7.2995.00050.0004.399.60.0000500.00005.000030.00003.000040	.1.65.2490.00009.00005.1.8.09996.0003000.00040.7.29950.00050.0004.399.6.00010.0000500.00005.6.000030.00003.000040.1	.1.65.2490.00009.000050.1.8.09996.000300.00010.00040.7.29950.0001.00050.0004.399.6.000100.0000500.00005.6.2499.000030.00004.000040.1.8	.1.65.2490.00009.000050.00005.1.8.09996.000300.000100.00040.7.29950.00010.00050.0004.399.6.0001000.000500.0005.6.2499.15.00030.0003.00040.1.8.0999

н.

TP3					
0.4 5.0 <i>E</i> – 07 5.0 <i>E</i> – 07	1.0 <i>E</i> – 07 0.3 0 0 3.0 <i>E</i> – 07	0 0.9999999 0	0 0 0.999999	0.3 5.0 <i>E</i> – 07 5.0 <i>E</i> – 07].

TP4 variants: TP41 $\equiv \varepsilon$ = 1.0E-01, TP42 $\equiv \varepsilon$ = 1.0E-03,											
TP43 $\equiv \varepsilon$ = 1.0E-05, TP44 $\equiv \varepsilon$ = 1.0E-07.											
		0	1	C	2		0	0	0		1
	.1– <i>ε</i>	.3	. 1	.2	.0	ε	0	0	U	0	
	.2	.1	.1	.2	.4	0	0	0	0	0	
	.1	.2	.2	.4	.1	0	0	0	0	0	
	.4	.2	.1	.2	.1	0	0	0	0	0	
	.6	.3	0	0	.1	0	0	0	0	0	
	Е	0	0	0	0	.1– <i>ε</i>	.2	.2	.4	.1	
	0	0	0	0	0	.2	.2	.1	.3	.2	
	0	0	0	0	0	.1	.5	0	.2	.2	
	0	0	0	0	0	.5	.2	.1	0	.2	
	0	0	0	0	0	.1	.2	.2	.3	.2	

15. Computational Comparisons

We present comparisons for the test problems, using GTH, Standard, Simple, Perturbation and Extended GTH procedures, under double precision, for the the stationary distribution and the MFPT matrix M

Comparisons are based upon computation of the the MAX RESIDUAL ERRORS:

MAX RES ERROR STAT DISTRN = $\max_{1 \le j \le m, j} \left| \hat{\pi}_{j} - \sum_{i} \hat{\pi}_{i} p_{ij} \right|$

MAX RES ERROR MFPT = $\max_{1 \le i \le m, 1 \le j \le m} \hat{m}_{ij} - \sum_{k \ne j} p_{ik} \hat{m}_{kj} - 1$

