AUT UNIVERSITY COMPUTER + MATHEMATICAL SCIENCES

The accurate computation of key properties of Markov and semi-Markov Processes

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1. Introduction

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

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

We are interested in developing accurate ways of finding two key properties of such chains:

(i) the stationary probabilites $\{\pi_j\}$, $(1 \leq j \leq N)$.

(ii) the mean first passage times $\{m_{ij}\}$,$(1 \leq i, j \leq N)$.

2. Stationary distributions

Let $\boldsymbol{\pi}^T = (\pi_1, \pi_2, \ldots, \pi_N)$ be the stationary prob. vector of the Markov chain with transition matrix $P = [p_{ij}]$.

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

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

3. Mean first passage times

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 $m_{ij} = E[T_{ij} \mid X_0 = i]$, the mean first passage time from state i to state j.

The mean first passage times

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

It is well known that

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

with $m_{jj} = 1/\pi_j$.

M satisfies the matrix equation

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

where $E = [1] = \mathbf{e}\mathbf{e}^T$, and

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

4. Solving for the stationary distribution

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

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

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

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

5. Solving for mean first passage times

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

$M = [G\Pi - E(G\Pi)_d + I - G + EG_d]D.$ (Hunter, 1982)

(ii) If $G\mathbf{e} = g\mathbf{e}$ for some g

$\Leftrightarrow M = [I - G + EG_d]D.$ (Hunter,2013)

The "**standard algorithm**" is $M = [I - Z + EZ_d]D$ where

Z= $[I - P + \mathbf{e}\boldsymbol{\pi}^T]^{-1}$, Kemeny and Snell's "fundamental matrix"

Solving for mean first passage times

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

If $G_{eb} = [I - P + \mathbf{e}\mathbf{e}_b^T]^{-1} = \left[g_{ij} \right],$

then $\pi_j = g_{bj}, \quad j = 1, 2, \ldots, N,$

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

Solving for mean first passage times

Hunter (2014) developed a variety "**perturbation algorithms**" where the transition matrix is successively updated row by row from an initial simple transition matrix to end up with the required transition matrix. One such algorithm is the following:

(i) Let $K_0 = I$.

(ii) For $i = 1,\ 2,\ \ldots, N$, let $\boldsymbol{p}_i^T = \boldsymbol{e}_i^T P,\ \boldsymbol{b}_i^T = \boldsymbol{p}_i^T - \ \boldsymbol{e}^T / N$,

$$K_i = K_{i-1}\left(I + C_i\right), where\ k_i = 1 - \boldsymbol{b}_i^T K_{i-1}\boldsymbol{e}_i\ \ and\ \ C_i = \frac{1}{k_i}\boldsymbol{e}_i \boldsymbol{b}_i^T K_{i-1}.$$

(iii) At $i = N$, let $K = K_N$ then $\boldsymbol{\pi}^T = \dfrac{1}{N}\boldsymbol{e}^T K,$

$$M = [I - K + EK_d]D, \text{ where } D = (\Pi_d)^{-1}\ .$$

6. 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. $\{X_k, k \geq 0\}$ with state space $S_N = \{1,2,...,N\}$, and transition probabilities $p_{ij}^{(N)} = P\{X_{k+1} = j \mid X_k = i\}$.

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 $S_N = S_{N-1} \cup \{N\},\ S_{N-1} = S_{N-2} \cup \{N-1\},....,\ S_2 = \{1,2\}$.

Once we get to two states we expand the state space one state at a time until we return to the final set S_N

Assume that the initial M.C. with state space S_N is irreducible and that stationary probability vector is given by $\boldsymbol{\pi}^T = (\pi_1, \pi_2, \ldots, \pi_{N-1}, \pi_N)$

Let $\boldsymbol{\pi}^T = \boldsymbol{\pi}^{(N)T} = (\pi_1^{(N)}, \pi_2^{(N)}, \ldots, \pi_{N-1}^{(N)}, \pi_N^{(N)})$.

From the stationary equations $\boldsymbol{\pi}^{(N)T} = \boldsymbol{\pi}^{(N)T} P_N$ or in element form $\pi_j^{(N)} = \sum_{i=1}^{N} \pi_i^{(N)} p_{ij}^{(N)} \quad (j = 1, 2, \ \ldots, N)$ express $\pi_N^{(N)}$ in terms of $\pi_1^{(N)}, \ldots, \ \pi_{N-1}^{(N)}$:

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

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

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

Partition the stationary probability vector

$\boldsymbol{\pi}^{(N)T} = (\boldsymbol{v}^{(N-1)T},\ \pi_N^{(N)})$ where $\boldsymbol{v}^{(N-1)T} = (\pi_1^{(N-1)}, \pi_2^{(N-1)}, \ldots, \pi_{N-1}^{(N-1)})$

It is easily shown that

$$\boldsymbol{v}^{(N-1)T}\left(I_{N-1} - P_{N-1}\right) = \boldsymbol{0}^T, \text{ where } P_{N-1} = Q_{N-1}^{(N)} - \frac{\boldsymbol{p}_{N-1}^{(N)(c)}\boldsymbol{p}_{N-1}^{(N)(r)T}}{\boldsymbol{p}_{N-1}^{(N)(r)T}\boldsymbol{e}^{(N-1)}}.$$

$$\text{Let } P_{N-1} = \left[p_{ij}^{(N-1)}\right] \text{ then } p_{ij}^{(N-1)} = p_{ij}^{(N)} + \frac{p_{iN}^{(N)}p_{Nj}^{(n)}}{S(N)},$$

$$1 \le i \le N-1,\ 1 \le j \le N-1$$

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

Observe

P_{N-1} is a stochastic matrix with state space S_{N-1}

P_{N-1} is irreducible

$\boldsymbol{v}^{(N-1)T}$ is a scaled stationary prob vector of this $N-1$ state MC

$$\boldsymbol{\pi}^{(N-1)T} = (\pi_1^{(N-1)}, \pi_2^{(N-1)}, \dots, \pi_{N-1}^{(N-1)}) \equiv \frac{1}{1-\pi_N^{(N)}} \boldsymbol{v}^{(N-1)T}$$

so that the first $N-1$ stationary probs of the N-state MC are scaled versions of the $N-1$ state MC.

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

Interpretation of the transition probabilities

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

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}.

For $(i,j) \in S_{n-1} \times S_{n-1}$ it is possible to jump directly from i to j with probability $p_{ij}^{(n)}$. Alternatively jump from i to j via state n, being held at state n for t (= 0,1,2,…) steps, followed by a jump to j, with probability

$$p_{in}^{(n)} \left(\sum_{t=0}^{\infty} \left(p_{nn}^{(n)} \right)^t \right) p_{nj}^{(n)} = \frac{p_{in}^{(n)} p_{nj}^{(n)}}{1 - p_{nn}^{(n)}} = \frac{p_{in}^{(n)} p_{nj}^{(n)}}{S(n)},$$

leading to the general expression for $p_{ij}^{(n-1)}$.

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

$$\boldsymbol{\pi}^{(N)T} = (\pi_1^{(N)}, \pi_2^{(N)}, \ldots., \pi_{N-1}^{(N)}, \pi_N^{(N)}) \equiv (\pi_1, \pi_2, \ldots., \pi_{n-1}, \pi_n)$$

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 $\pi_1, \pi_2, \ldots., \pi_{n-1}$.

Thus each $\boldsymbol{\pi}^{(n)T}$ is a scaled version of $(\pi_1, \pi_2, \ldots., \pi_{n-1}, \pi_n)$.

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 $\boldsymbol{\pi}^{(2)T} = (\pi_1^{(2)}, \pi_2^{(2)})$ 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 $S(2) = 1 - p_{22}^{(2)} = \sum_{j=1}^{1} p_{2j}^{(2)} = p_{21}^{(2)} = \boldsymbol{p}_1^{(2)(r)T} e^{(1)}$.

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, $\pi_n = \dfrac{\sum_{i=1}^{n-1} \pi_i p_{in}^{(n)}}{\sum_{i=1}^{n-1} p_{ni}^{(n)}} = \sum_{i=1}^{n-1} \pi_i \dfrac{p_{in}^{(n)}}{S(n)}$

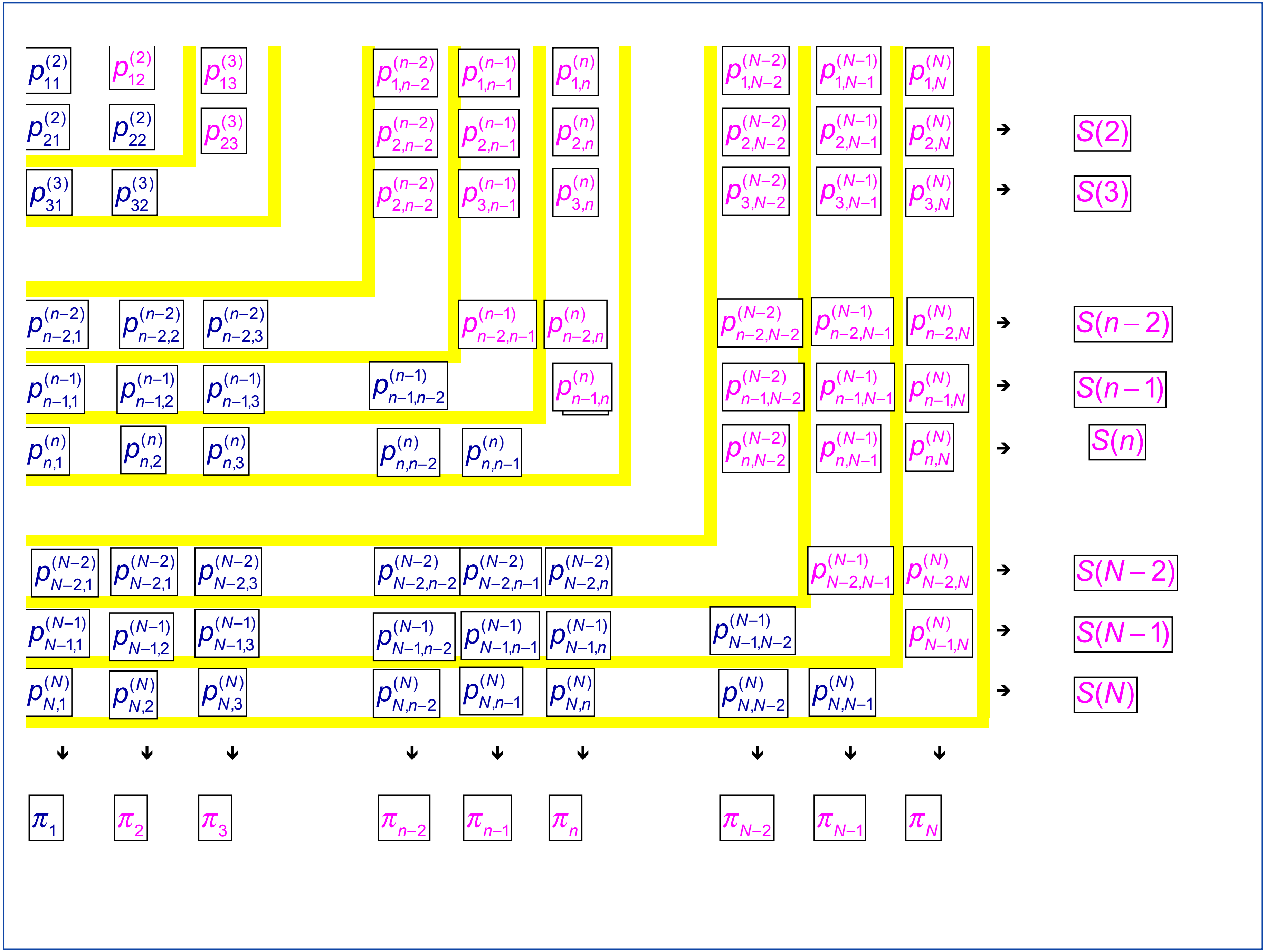
If $\pi_j = kr_j$ with $r_1 = 1$ then

$\sum_{i=1}^{N} \pi_i = 1 \Rightarrow k = 1 \Big/ \sum_{i=1}^{N} r_i$ with

$$r_n = \frac{\sum_{i=1}^{n-1} r_i p_{in}^{(n)}}{S(n)}, (n = 2, \ldots, N),$$

implying

$$\pi_i = \frac{r_i}{\sum_{n=1}^{N} r_n}, \quad i = 1, 2, \ldots, N.$$


$p_{11}^{(2)}$ $p_{12}^{(2)}$ $p_{13}^{(3)}$ $p_{1,n-2}^{(n-2)}$ $p_{1,n-1}^{(n-1)}$ $p_{1,n}^{(n)}$ $p_{1,N-2}^{(N-2)}$ $p_{1,N-1}^{(N-1)}$ $p_{1,N}^{(N)}$
$p_{21}^{(2)}$ $p_{22}^{(2)}$ $p_{23}^{(3)}$ $p_{2,n-2}^{(n-2)}$ $p_{2,n-1}^{(n-1)}$ $p_{2,n}^{(n)}$ $p_{2,N-2}^{(N-2)}$ $p_{2,N-1}^{(N-1)}$ $p_{2,N}^{(N)}$ $S(2)$
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π_1 π_2 π_3 π_{n-2} π_{n-1} π_n π_{N-2} π_{N-1} π_N

GTH Algorithm

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

2. Compute for $n = N, N\!-\!1, \ldots, ,3,$

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

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

3. Set $r_1 = 1$ and compute $r_n = \dfrac{\sum_{i=1}^{n-1} r_i p_{in}^{(n)}}{S(n)}$, for $n = 2, \ldots, N$.

4. Compute $\pi_i = \dfrac{r_i}{\sum_{j=1}^{N} r_j}$, $i = 1, 2, \ldots, N$.

7. 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 $E = \left[1\right] = \boldsymbol{e}^{(N)}\boldsymbol{e}^{(N)T}$ and

$$M_d = \left[\delta_{ij} m_{jj}\right] = diag(\pi_1, \pi_2, \ldots, \pi_N).$$

For a M.R.P. $\{X_n, T_n\}$ the MFPT matrix satisfies

$$(I-P)M = \boldsymbol{\mu}^{(N)}\boldsymbol{e}^{(N)T} - P(M)_d.$$

M.R.P Primer

From Hunter (1982)

Let $\{(X_n, T_n)\}, (n \geq 0\}$, be a Markov renewal process (M.R.P.

with state space S_N and semi-Markov kernel $Q(t) = \left[Q_{ij}(t) \right]$,

where $Q_{ij}(t) = P\{X_{n+1} = j,\ T_{n+1} - T_n \leq t \mid X_n = i\},\ (i, j) \in S_N$.

X_n is the state at the n-th transition

T_n is the time of the *n*-th transition.

Let $P = \left[p_{ij} \right]$ be the transition matrix of the embedded

M.C. $\{ X_n\}, (n \geq 0),\ p_{ij} = Q_{ij}(+\infty) = P\{X_{n+1} = j \mid X_n = i\}$.

$Q_{ij}(t) = p_{ij} F_{ij}(t)$ where $F_{ij}(t) = P\{T_{n+1} - T_n \leq t \mid X_n = i,\ X_{n+1} = j\}$

$F_{ij}(t)$ 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 $\mu_{ij} = p_{ij} E[T_{n+1} - T_n \big| X_n = i,\ X_{n+1} = j]$.

Let $P^{(1)} = \left[\mu_{ij} \right]$ then

$$(I - P)M = P^{(1)}E - PM_d.$$

Let $\boldsymbol{\mu} = P^{(1)}\boldsymbol{e}$ then $\boldsymbol{\mu}^T = (\mu_1, \mu_2, \ldots, \mu_N)$ where $\mu_i = \sum_{j=1}^{N} \mu_{ij}$.

$\mu_i = E[T_{n+1} - T_n \big| X_n = i]$ is the "mean holding time in state i ".

Thus $P^{(1)}E = P^{(1)}\boldsymbol{e}\boldsymbol{e}^T = \boldsymbol{\mu}\boldsymbol{e}^T$

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

Let us partition $M = M_N$ as $M_N = \begin{bmatrix} M_{N-1} & \boldsymbol{m}_{N-1}^{(N)(c)} \\ \boldsymbol{m}_{N-1}^{(N)(r)T} & m_{NN} \end{bmatrix}$

where

$M_{N-1} = \left[m_{ij} \right]$, $(1 \le i \le N-1,\ 1 \le j \le N-1)$,

$\boldsymbol{m}_{N-1}^{(N)(r)T} = (m_{N1}, m_{N2}, \ldots., m_{N,N-1})$ and

$\boldsymbol{m}_{N-1}^{(N)(c)T} = (m_{1N}, m_{2N}, \ldots., m_{N-1,N})$.

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

where $\boldsymbol{\mu}_{N-1}^{(N)T} = (\mu_1^{(N)}, \ldots, \mu_{N-1}^{(N)})$

Expressing $(I - P)M = \boldsymbol{\mu}^{(N)} \boldsymbol{e}^{(N)T} - P(M)_d$ 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

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

where $$\boldsymbol{\mu}^{(N-1)} = \boldsymbol{\mu}_{N-1}^{(N)} + \frac{\mu_N^{(N)}\boldsymbol{p}_{N-1}^{(N)(c)}}{\boldsymbol{p}_{N-1}^{(N)(r)T}\boldsymbol{e}^{(N-1)}}.$$

Further, $$\boldsymbol{m}_{N-1}^{(N)(r)T} = \frac{\left\{\boldsymbol{p}_{N-1}^{(N)(r)T}\left(M_{N-1} - (M_{N-1})_d\right) + \mu_N^{(N)}\boldsymbol{e}^{(N-1)T}\right\}}{\boldsymbol{p}_{N-1}^{(N)(r)T}\boldsymbol{e}^{(N-1)}}$$

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 $\boldsymbol{m}_{N-1}^{(N)(c)}$, i.e. the m_{iN} for $1 \le i \le N-1$.

$$(I_{n-1} - Q_{n-1}^{(n)})\boldsymbol{m}_{n-1}^{(n)(c)} = \boldsymbol{\mu}_{n-1}^{(n)}$$

$Q_{N-1}^{(N)} = \left[p_{ij}^{(N)} \right]$ 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 $m_{N-1,N}$ from $\boldsymbol{m}_{N-1}^{(N)(c)T}$ replacing it in the expressions for the elements $m_{1N}, m_{2N}, \ldots, m_{N-2,N}$.

Need to express $(N-1)\times(N-1)$ matrix $Q_{N-1}^{(N)}$ in block form.

$$m_{N-1,N} = \frac{\left\{ \boldsymbol{p}_{N-2}^{(N-1)(N)(r)T} \boldsymbol{m}_{N-2}^{(N)(c)} + \mu_{N-1}^{(N)} \right\}}{1 - p_{N-1,N-1}^{(N-1)}} = \frac{\left\{ \sum_{k=1}^{N-2} q_{N-1,k}^{(N-1)} m_{kN} + \mu_{N-1}^{(N)} \right\}}{R(N)},$$

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 $(I_n - P_n)M_n = \boldsymbol{\mu}^{(n)}\boldsymbol{e}^{(n)T} - P_n(M_n)_d$ where $\boldsymbol{\mu}^{(n)T} = (\boldsymbol{\mu}_{n-1}^{(n)}, \mu_n^{(n)})$,

then $(I_{n-1} - P_{n-1})M_{n-1} = \boldsymbol{\mu}^{(n-1)}\boldsymbol{e}^{(n-1)T} - P_{n-1}(M_{n-1})_d$

where $\boldsymbol{\mu}^{(n-1)T} = \boldsymbol{\mu}_{n-1}^{(n)T} + \dfrac{\mu_n^{(n)}\boldsymbol{p}_{n-1}^{(n)(c)T}}{\boldsymbol{p}_{n-1}^{(n)(r)T}\boldsymbol{e}^{(n-1)}}$.

$\boldsymbol{\mu}^{(n)T} = (\boldsymbol{\mu}_{n-1}^{(n)T}, \mu_n^{(n)})$ is a $1\times n$ vector, $\boldsymbol{\mu}_{n-1}^{(n)T} = (\mu_1^{(n)},\ldots,\mu_{n-1}^{(n)})$ and

$\boldsymbol{\mu}^{(n-1)T} = (\mu_1^{(n-1)},\ldots,\mu_{n-1}^{(n-1)})$ is a $1\times(n-1)$ 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 $S(n) = \boldsymbol{p}_{n-1}^{(n)(r)T}\boldsymbol{e}^{(n-1)} = \sum_{j=1}^{n-1} p_{nj}^{(n)} = 1 - p_{nn}^{(n)}$.

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. $M_{n-1} = \left[m_{ij} \right]$, 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 $M_{n-1} = \left[m_{ij} \right]$, $(1 \le i \le n-1,\ 1 \le j \le n-1)$,

we wish to find $\boldsymbol{m}_{n-1}^{(n)(c)}, \boldsymbol{m}_{n-1}^{(n)(r)T}$ 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 $\boldsymbol{m}_{n-1}^{(n)(c)}$, $m_{nj} = \dfrac{\left\{ \sum_{k=1, k \ne j}^{n-1} p_{nk}^{(n)} m_{kj} + \mu_n^{(n)} \right\}}{S(n)}$ for $1 \le j \le n-1$.

For $n = 2$: $$(I_2 - P_2)M_2 = \boldsymbol{\mu}^{(2)}\boldsymbol{e}^{(2)T} - P_2(M_2)_d$$

$$\begin{bmatrix} 1-p_{11}^{(2)} & -p_{12}^{(2)} \\ -p_{21}^{(2)} & 1-p_{22}^{(2)} \end{bmatrix}\begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}$$

$$= \begin{bmatrix} \mu_1^{(2)} & \mu_1^{(2)} \\ \mu_2^{(2)} & \mu_2^{(2)} \end{bmatrix} - \begin{bmatrix} p_{11}^{(2)}m_{11} & p_{12}^{(2)}m_{22} \\ p_{21}^{(2)}m_{11} & p_{22}^{(2)}m_{22} \end{bmatrix}$$

leading to

$$M_2 = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} = \begin{bmatrix} \dfrac{p_{21}^{(2)}\mu_1^{(2)} + p_{12}^{(2)}\mu_2^{(2)}}{p_{21}^{(2)}} & \dfrac{\mu_1^{(2)}}{p_{12}^{(2)}} \\ \dfrac{\mu_2^{(2)}}{p_{21}^{(2)}} & \dfrac{p_{21}^{(2)}\mu_1^{(2)} + p_{12}^{(2)}\mu_2^{(2)}}{p_{12}^{(2)}} \end{bmatrix}$$

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 $p_{ij}^{(n-1)} = p_{ij}^{(n)} + \dfrac{p_{in}^{(n)} p_{nj}^{(n)}}{S(n)},\quad 1 \le i \le n-1,\ 1 \le j \le n-1$

and $\mu_i^{(n-1)} = \mu_i^{(n)} + \dfrac{\mu_n^{(n)} p_{i,n}^{(n)}}{S(n)},\ (1 \le i \le n - 1),$ with $S(n) = \sum_{j=1}^{n-1} p_{nj}^{(n)}$.

with $(\mu_1^{(N)}, \mu_2^{(N)}, ..., \mu_N^{(N)}) = (1,1,...,1).$

Let $m_{11} = \mu_1^{(2)} + \dfrac{p_{12}^{(2)}\mu_2^{(2)}}{p_{21}^{(2)}}$,

$$m_{21} = \frac{\mu_2^{(2)}}{S(2)},$$

$$m_{31} = \frac{p_{32}^{(3)} m_{21} + \mu_3^{(3)}}{S(3)},$$

$$m_{n1} = \frac{\sum_{k=2,}^{n-1} p_{nk}^{(n)} m_{k1} + \mu_n^{(n)}}{S(n)}, \; n = 3,\ldots,N.$$

This provides the entries of the first column of $M = \left[m_{ij} \right]$, i.e. $\boldsymbol{m}_N^{(1)(N)}$, where

$M = \ (\boldsymbol{m}_N^{(1)(N)}, \boldsymbol{m}_N^{(2)(N)} \ldots, \boldsymbol{m}_N^{(N)(N)})$ with $\boldsymbol{m}_N^{(1)(N)T} = (m_{11}, m_{21}, \ldots, m_{N1})$

$$
\begin{matrix}
m_{11} & m_{12} & m_{13} & m_{14} & m_{15} \\
m_{21} & m_{22} & m_{23} & m_{24} & m_{25} \\
m_{31} & m_{32} & m_{33} & m_{34} & m_{35} \\
m_{41} & m_{42} & m_{43} & m_{44} & m_{45} \\
m_{51} & m_{52} & m_{53} & m_{54} & m_{55}
\end{matrix}
$$

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

$$P_N \equiv P_N^{(1)} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1,N-1} & p_{1,N} \\ p_{21} & p_{22} & & p_{2,N-1} & p_{2N} \\ & & & & \\ p_{N-1.1} & p_{N-1,2} & & p_{N-1,N-1} & p_{N-1,N} \\ p_{N1} & p_{N2} & & p_{N,N-1} & p_{NN} \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} p_{22} & p_{2,N-1} & p_{2N} & p_{21} \\ & & & \\ p_{N-1,2} & p_{N-1,N-1} & p_{N-1,N} & p_{N-1,1} \\ p_{N2} & p_{N,N-1} & p_{NN} & p_{N.1} \\ p_{12} & p_{1,N-1} & p_{1,N} & p_{11} \end{bmatrix} \equiv P_N^{(2)}$$

Step 3: Carry out the algorithm, as in Step 1, with $P_N = P_N^{(2)}$

to obtain the vector of MFPTs which we label as $\overline{\boldsymbol{m}_N}^{(2)(N)}$

where $\overline{\boldsymbol{m}_N}^{(2)(N)T} = (m_{22}, m_{32}, \ldots., m_{N2}, m_{12})$.

Step 4: Reorder $P_2^{(N)}$ as in step 2 to obtain $P_3^{(N)}$ and repeat Step 3

to obtain $\overline{\boldsymbol{m}}^{(3)(N)}$ where $\overline{\boldsymbol{m}}^{(3)(N)T} = (m_{33}, m_{43}, \ldots, m_{N3}, m_{13}, m_{23})$

Step k: Repeat as above with $P_k^{(N)}$ to obtain $\overline{\boldsymbol{m}}^{(k)(N)}$ where

$\overline{\boldsymbol{m}}^{(k)(N)T} = (m_{kk}, m_{k+1,k}, \ldots, m_{N,k}, m_{1,k}, \ldots, m_{k-1,k})$ finishing with

$P_N^{(N)}$ and $\overline{\boldsymbol{m}}^{(N)(N)}$ where $\overline{\boldsymbol{m}}^{(N)(N)T} = (m_{NN}, m_{1,N}, m_{2,N}, \ldots, m_{N-1,N})$

Step $N+1$: Let $\overline{M} = (\boldsymbol{m}_N^{(1)(N)}, \overline{\boldsymbol{m}_N}^{(2)(N)} \ldots., \overline{\boldsymbol{m}_N}^{(N)(N)})$

Finally reorder $\overline{M}$ to obtain $M = (\boldsymbol{m}_N^{(1)(N)}, \boldsymbol{m}_N^{(2)(N)} \ldots., \boldsymbol{m}_N^{(N)(N)})$

This can be carried out using the following MatLab procedure:

```
    end
       for col=1:m
           for row= 1:m
           P_new1(mod(row+m-2,m)+1,col)=P(row,col);
           end
       end
       for col=1:m
           for row= 1:m
          P_new2(row,mod(col+m-2,m)+1)=P_new1(row,col);
           end
       end
      P=P_new2;
       PP=P;
   end
   for col=1:m
       for row=1:m
           M1(mod(row+col-2,m)+1,col)=M(row,col);
       end
```

8. 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

$$\begin{bmatrix} .1 & .6 & 0 & .3 & 0 & 0 \\ .5 & .5 & 0 & 0 & 0 & 0 \\ .5 & .2 & 0 & 0 & .3 & 0 \\ 0 & .7 & 0 & .2 & 0 & .1 \\ .1 & 0 & .8 & 0 & 0 & .1 \\ .4 & 0 & .4 & 0 & 0 & .2 \end{bmatrix}$$

TP2 (Also Benzi (2004))

$$\begin{bmatrix} .85 & 0 & .149 & .0009 & 0 & .00005 & 0 & .00005 \\ .1 & .65 & .249 & 0 & .00009 & .00005 & 0 & .00005 \\ .1 & .8 & .09996 & .0003 & 0 & 0 & .0001 & 0 \\ 0 & .0004 & 0 & .7 & .2995 & 0 & .0001 & 0 \\ .0005 & 0 & .0004 & .399 & .6 & .0001 & 0 & 0 \\ 0 & .00005 & 0 & 0 & .00005 & .6 & .2499 & .15 \\ .00003 & 0 & .00003 & .00004 & 0 & .1 & .8 & .0999 \\ 0 & .00005 & 0 & 0 & .00005 & .1999 & .25 & .55 \end{bmatrix}.$$

TP3

$$\begin{bmatrix} 0.999999 & 1.0\,E-07 & 2.0\,E-07 & 3.0\,E-07 & 4.0\,E-07 \\ 0.4 & 0.3 & 0 & 0 & 0.3 \\ 5.0\,E-07 & 0 & 0.999999 & 0 & 5.0\,E-07 \\ 5.0\,E-07 & 0 & 0 & 0.999999 & 5.0\,E-07 \\ 2.0\,E-07 & 3.0\,E-07 & 1.0\,E-07 & 4.0\,E-07 & 0.999999 \end{bmatrix}.$$

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.

$$\begin{bmatrix} .1-\varepsilon & .3 & .1 & .2 & .3 & \varepsilon & 0 & 0 & 0 & 0 \\ .2 & .1 & .1 & .2 & .4 & 0 & 0 & 0 & 0 & 0 \\ .1 & .2 & .2 & .4 & .1 & 0 & 0 & 0 & 0 & 0 \\ .4 & .2 & .1 & .2 & .1 & 0 & 0 & 0 & 0 & 0 \\ .6 & .3 & 0 & 0 & .1 & 0 & 0 & 0 & 0 & 0 \\ \varepsilon & 0 & 0 & 0 & 0 & .1-\varepsilon & .2 & .2 & .4 & .1 \\ 0 & 0 & 0 & 0 & 0 & .2 & .2 & .1 & .3 & .2 \\ 0 & 0 & 0 & 0 & 0 & .1 & .5 & 0 & .2 & .2 \\ 0 & 0 & 0 & 0 & 0 & .5 & .2 & .1 & 0 & .2 \\ 0 & 0 & 0 & 0 & 0 & .1 & .2 & .2 & .3 & .2 \end{bmatrix}$$

9. Comparisons

We present comparisons for the test problems, the 4 algorithms (Standard, Simple, Perturbations and Extended GTH), under double precision, for the MFPT matrix M and compute the MAX RESIDUAL ERRORS:

$$\text{MAX RES ERROR} = \max_{1 \le i \le m, 1 \le j \le m} \left| m_{ij} - \sum_{k \ne j} p_{ik} m_{kj} - 1 \right|$$

Max Res Error	M_Standard	M_Simple	M_Pert	M_EGTH
TP1	5.6843e-14	5.6843e-14	1.1369e-13	1.1369e-13
TP2	1.8190e-12	1.8190-12	3.6380e-12	3.6380e-12
TP3	1.7027	1.7594	1.5073	1.6188
TP41	1.4211e-14	2.1316e-14	1.4211e-14	1.4211e-14
TP42	1.0374e-12	1.8190e-12	9.0950e-13	1.8190e-12
TP43	1.1642e-10	1.7462e-10	1.7462e-10	1.1642e-10
TP44	1.4901e-08	1.4901e-08	1.4901e-08	7.4506e-09