Efficient Computation of Equilibrium/Transient Probability Distribution of Arbitrary Finite State Space Continuous Time Markov Chains

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Abstract. In this research paper, efficient algorithms for computation of equilibrium as well as transient probability distribution of arbitrary finite state space Continuous / Discrete Time Markov Chains are proposed. The effective idea is to solve a structured systems of linear equations efficiently. The ideas of this research paper could be utilized in solving structured system of linear equations that arise in other applications.

Keywords: Continuous Time Markov Chains · Region of Convergence · Generator Matrix

1 Introduction

Markov chains provide interesting stochastic models of natural/artificial phenomena arising in science and engineering. The existence of equilibrium behavior enables computation of equilibrium performance measures. Thus, researchers invested considerable effort in efficiently computing the equilibrium probability distribution of Markov Chains and thus, the equilibrium performance measures.

Traditionally, computation of transient probability distribution of Continuous Time Markov Chains (CTMCs) was considered to be a difficult open problem. It requires computation of Matrix Exponential associated with the generator matrix of CTMC. Even in the case of finite state space CTMCs, efficient computation of transient probability distribution was considered to be a difficult open problem. In [5], an interesting approach for recursive computation of transient probability distribution of arbitrary finite state space CTMCs was proposed. In the case of infinite state space, Quasi-birth-and-Death (QBD) processes, matrix geometric recursion for transient probability distribution was found in [16].

It is well known that computation of equilibrium distribution of CTMCs reduces to solution of linear system of equations. The approach proposed in [6] reduces the computation of transient probability distribution of finite state space CTMCs to solving linear system of equations in the transform (Laplace transform) domain. Thus, an interesting question that remained deals with efficient solution of such structured linear system of equations in the Laplace transform

domain. In fact, a more interesting problem is to design an algorithm which meets a lower bound on the computation of solution of structured system of linear equations arising in the transient/equilibrium analysis of CTMCs.

This research paper is organized as follows. In Section 2, related literature is reviewed. In Section 3, algorithm for efficient computation of equilibrium probability mass function (PMF) of CTMCs is discussed. In Section 4, algorithm for efficient computation of transient PMF of CTMCs is discussed. In Section 5, we provide numerical results. The research paper concludes in Section 6.

2 Review of Literature

It is well known that computation of equilibrium probability vector $\bar{\pi}$ of a Homogeneous CTMC with generator Q reduces to the solution of the following linear system of equations (computation of vector $\bar{\pi}$ in the left null space of the generator matrix Q):

$$\bar{\pi}Q \equiv \bar{0}.$$

It should be noted that in the case of homogeneous Discrete Time Markov Chain (DTMC) with state transition matrix $\bar{P}$, the computation of equilibrium probability vector $\bar{\pi}$ reduces to the solution of following linear system of equations i.e.

$$\bar{\pi}\bar{P} \equiv \bar{\pi} \text{ or, equivalently, } \bar{\pi}(\bar{P} - I) \equiv \bar{0}.$$

It readily follows that $(\bar{P} - I)$ has the properties of a generator matrix. Thus, in the following discussion, we consider only the computation of equilibrium probability vector of a CTMC. In computational linear algebra, there are efficient algorithms to solve linear system of equations [3], [12], [15]. Volker Strassen made fundamental contributions to this problem [13], [14]. He showed that the complexity of matrix inversion is equivalent to that of matrix multiplication. It readily follows that the matrix $-Q$ is a Laplacian matrix (i.e. a square matrix with positive diagonal and non-positive off-diagonal elements such that the row sums are zero). There are efficient algorithms to solve Laplacian system of equations [1], [2].

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But, from the point of view of computing $\bar{\pi}$, the structure of generator matrix Q was not completely taken into account. Thus, the goal of this research paper is to design efficient algorithm for computing $\bar{\pi}$, taking into account the structure of generator matrix Q. Some related effort dealing with Laplacian system of equations is discussed in [2]. In fact, we would like to design a computationally optimal algorithm for computation of $\bar{\pi}$ (in terms of computational complexity). We illustrate the essential idea with a CTMC with 4 states.

3.1 CTMC with 4 States

First consider the generator matrix of a CTMC with 4 states (i.e. 4 x 4 matrix) partitioned using blocks of size 2 x 2 (i.e. there are 4 such 2 x 2 matrices in the generator) [9], [10]. Specifically, we have

$$Q = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \tag{1}$$

where $A_{i,j}$, $i, j \in \{1, 2\}$, are 2 x 2 square matrices in the 4 x 4 block matrix Q.

Claim: For an irreducible positive recurrent (recurrent non-null) CTMC with generator matrix Q, it is well known that the matrices A_{11} and A_{22} are non-singular. Hence, we have that

$$A_{21} = A_{22}X \text{ with } X = A_{22}^{-1}A_{21}.$$

Thus, by means of elementary column operations (i.e. multiplication by a scalar and addition/subtraction), the generator matrix Q can be converted into the block upper triangular form:

$$\tilde{Q} = \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ 0 & A_{22} \end{bmatrix}. \tag{2}$$

Note that $\tilde{A}_{22} = A_{22}$.

Let $X = [f_1 \ f_2]$. Hence, column operations to arrive at $\tilde{Q}$ (from Q) are determined by the column vectors f_1, f_2. Also, it follows from linear algebra, that the equilibrium probability vector $\bar{\pi}$ is unaffected by such column operations. Hence, with $\bar{\pi} = [\bar{\pi}_1 \ \bar{\pi}_2]$, we have the following system of linear equations:

$$\bar{\pi}_1 \tilde{A}_{11} = \bar{0},$$

i.e. the boundary system of two equations and

$$\bar{\pi}_1 \tilde{A}_{12} + \bar{\pi}_2 A_{22} = \bar{0}.$$

Thus, we have

$$\bar{\pi}_2 = -\bar{\pi}_1 \tilde{A}_{12} A_{22}^{-1}.$$

The boundary system of equations corresponds to a singular matrix $\tilde{A}_{11}$ for an irreducible, recurrent non-null Markov chain (otherwise $\bar{\pi}$ will be zero). Thus the boundary system of linear equations leads to a single linear equation in two variables $\bar{\pi}_1 = [\pi_{1,1} \ \pi_{1,2}]$. Hence we have a linear equation of the form

$$\pi_{1,1}\alpha + \pi_{1,2}\beta = 0. \text{ Thus, } \pi_{1,2} = -\pi_{1,1}\frac{\alpha}{\beta}.$$

Further, since $\bar{\pi}_2$ can be expressed in-terms of $\bar{\pi}_1$, we utilize the normalizing equation

$$\bar{\pi}\bar{e} = 1,$$

where $\bar{e}$ is a column vector of ones, to determine $\pi_{1,1}$ and hence all the other equilibrium probabilities.

Remark 1: We realize that the inverse of a 2 x 2 matrix can be computed by inspection and essentially only requires computation of the determinant. For instance, let us consider a 2 x 2 matrix B:

$$B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}. \tag{3}$$

It is well known that

$$B^{-1} = \frac{1}{\Delta} \begin{bmatrix} b_{22} & -b_{12} \\ -b_{21} & b_{11} \end{bmatrix}, \tag{4}$$

where

$$\Delta = \det(B) = (b_{11}b_{22} - b_{12}b_{21}).$$

Computational Complexity Now we determine the computational complexity of our algorithm:

- The number of arithmetic operations required to convert the generator matrix Q into block upper triangular matrix $\tilde{Q}$ are as follows. We need one 2 x 2 matrix inversion, one 2 x 2 matrix multiplication and one addition of 2 x 2 matrices.
- π_1^2 computation requires one division.
- π_2 computation requires inversion of 2 x 2 matrix A_{22} and one matrix multiplication (of 2 x 2 matrices $\tilde{A}_{12}$ and A_{22}).
- Also, the normalizing equation to determine $\pi_{1,1}$ requires 3 additions and one division.
- Finally, to determine $\bar{\pi}_1$, $\bar{\pi}_2$ in terms of $\pi_{1,1}$, we require 3 multiplications.

3.2 CTMC with Arbitrary Finite Number of States

Now, we generalize the above algorithm for the case, where the number of states, $N = 2m$, where $m > 2$. In such case, the generator matrix is of the following form:

$$Q = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1m} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2m} \\ A_{31} & A_{32} & A_{33} & \cdots & A_{3m} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ A_{m1} & A_{m2} & A_{m3} & \cdots & A_{mm} \end{bmatrix},$$

where $A_{ij}, i, j = 1, \ldots, m$, are 2 x 2 matrices.

Lemma 1: For a positive recurrent CTMC, the following sub-matrices of generator i.e.

$$\{A_{ii} : 1 \leq i \leq m\}$$

are all non-singular matrices, except A_{11} or A_{mm}.

Proof: Refer [5]. The proof utilizes the fact that strictly diagonally dominant matrix is non-singular. □

Hence, as in the $m = 2$ case, by means of elementary column operations on the generator matrix Q, we arrive at the following block upper triangular matrix $\tilde{Q}$.

$$\tilde{Q} = \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} & \tilde{A}_{13} & \cdots & \tilde{A}_{1m-1} & \tilde{A}_{1m} \\ 0 & \tilde{A}_{22} & \tilde{A}_{23} & \cdots & \tilde{A}_{2m-1} & \tilde{A}_{2m} \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \tilde{A}_{m-1m-1} & \tilde{A}_{m-1m} \\ 0 & 0 & 0 & \cdots & 0 & A_{mm} \end{bmatrix}.$$

Thus, the equilibrium probability vector $\bar{\pi}$ satisfies the following linear system of equations:

$$\bar{\pi}_1 \tilde{A}_{12} \equiv \bar{0}$$
$$\bar{\pi}_1 \tilde{A}_{12} + \bar{\pi}_2 \tilde{A}_{22} \equiv \bar{0}.$$
$$\vdots$$
$$\bar{\pi}_1 \tilde{A}_{1m-1} + \bar{\pi}_2 \tilde{A}_{2m-1} + \cdots + \bar{\pi}_{m-1} \tilde{A}_{m-1m-1} \equiv \bar{0}$$
$$\bar{\pi}_1 \tilde{A}_{1m} + \bar{\pi}_2 \tilde{A}_{2m} + \cdots + \bar{\pi}_m A_{mm} \equiv \bar{0}.$$

The above system of linear equations is recursively solved to compute the equilibrium probability vector i.e.

$$\bar{\pi}_1 \tilde{A}_{11} \equiv \bar{0}$$
$$\bar{\pi_2} = -\bar{\pi}_1 \tilde{A}_{12} \tilde{A}_{22}^{-1}.$$
$$\vdots$$
$$\bar{\pi}_j = -\bar{\pi}_1 \tilde{A}_{1j} \tilde{A}_{jj}^{-1} - \bar{\pi}_2 \tilde{A}_{2j} \tilde{A}_{jj}^{-1} - \cdots - \bar{\pi}_{j-1} \tilde{A}_{j-1j} \tilde{A}_{jj}^{-1}$$

for $2 \leq j \leq (m-1)$,

$$\bar{\pi}_m = -\bar{\pi}_1 \tilde{A}_{1m} \tilde{A}_{mm}^{-1} - \bar{\pi}_2 \tilde{A}_{2m} \tilde{A}_{mm}^{-1} - \cdots - \bar{\pi}_{m-1} \tilde{A}_{m-1m} A_{mm}^{-1}.$$

As in the $m = 2$ case, using non-singular matrices on the diagonal of generator matrix, Q, it can be converted to a block upper-triangular matrix. Since inverse of 2 x 2 matrices on the diagonal of Q can be computed efficiently, an efficient algorithm exists for such a computational problem.

Definition: *finite memory recursion* of order L for the equilibrium probability vector is of the following form

$$\bar{\pi}(L+1) = \bar{\pi}(1)W_1 + \bar{\pi}(2)W_2 + \cdots + \bar{\pi}(L)W_L,$$

where $W_i, i = 1, \ldots, L$, are recursion matrices. We call such a recursion *forward finite memory recursion* [8]. Such a forward finite memory recursion holds true for infinite state space CTMCs also [5], [6], [8].

Remark 2: Since $\tilde{A}_{jj}$ are all non-singular 2 x 2 matrices, their inverse can be efficiently computed.

Computational Complexity We now compute the computational complexity of the algorithm to determine equilibrium probabilities in most general case.

- *Conversion of Q into a Block Upper Triangular Matrix:* This task is accomplished using an approach similar to Gaussian elimination using the 2 x 2 non-singular matrices. It requires
  (i)
  $$(M-1)^2 + (M-2)^2 + \cdots + 2^2 + 1 = \frac{M(M-1)(2M-1)}{6},$$
  2 x 2 matrix multiplication,
  $$\frac{M(M-1)(2M-1)}{6},$$
  2 x 2 matrix additions and $(M-1)$ inversions of 2 x 2 matrices.
  (ii) *2 x 2 Matrix inversions needed in Finite Memory Recursion:* We require $(m-2)$ inversions of 2 x 2 matrices (since $\tilde{A_{mm}}$ is already inverted in step (i)). Each 2 x 2 matrix inversion requires (a) Determinant computation i.e. 2 multiplications and one subtraction; (b) Division of elements by determinant i.e. 4 divisions.
  (iii) *2 x 2 Matrix Multiplications:* In the above system of linear equations, we require
  $$1 + 2 + 3 + \cdots + (m-1) = \frac{m(m-1)}{2}$$
  multiplications of two 2 x 2 matrices. Each such multiplication (of two 2 x 2 matrices) requires at most 8 multiplications and 4 additions. To reduce the complexity, we can utilize Strassen's multiplication algorithm. The number of multiplications required to compute the product of 2 x 2 matrices reduces to 7 (using Strassen's algorithm). But with Strassen's algorithm we require 18 additions/subtractions.
  (iv) *Vector Matrix Multiplications:* We require
  $$1 + 2 + 3 + \cdots + (m-1) = \frac{m(m-1)}{2}$$
  multiplications of 1 x 2 and 2 x 2 matrices (i.e. multiplication of row vector and 2 x 2 matrix).
- *Normalization* requires $(2m-1)$ additions and one division to obtain $\pi_{1,1}$.
- Finally, we require $(2m-1)$ multiplications to determine the equilibrium probabilities using π_1^1.

Thus, total number of 2 x 2 matrix inversions, 2 x 2 matrix multiplications and 2 x 2 matrix additions and other arithmetical operations required can be readily determined.

Note that in the computer implementation of any algorithm, divisions are "more expensive" than multiplications. Hence, in the above inversion of 2 x 2 matrices, we first compute the inverse of determinant Δ and convert the associated divisions to multiplications.

Note also that in the case of QBD processes, Latouche et.al utilize Gaussian Elimination method to compute the equilibrium probability distribution [4]. In fact they provide probabilistic interpretation of the method.

Remark 3: Suppose, the number of states of the CTMC is an Odd number. Then, we consider the 3 x 3 boundary system of linear equations (i.e. the initial probability vector is of dimension 3) and utilize the above idea to compute the equilibrium probability vector efficiently.

Remark 4: It should be noted that using similar idea (as discussed above), by means of elementary column operations, the generator matrix can be converted into a block lower triangular matrix. In this case, the boundary system of linear equations is at the trailing boundary. By solving for the last probability vector, we recursively compute the equilibrium probabilities. We call such a recursion as the *backward finite memory recursion* [5].

4 Efficient Computation of Transient Probability Mass Function of CTMCs

It is well known that the transient PMF of a homogeneous CTMC (generator matrix doesn't depend on time t, unlike non-homogeneous CTMC) satisfies the following vector matrix differential equation i.e.

$$\frac{d}{dt}\bar{\pi}(t) = \bar{\pi}(t)Q.$$

Taking Laplace-Transform on both sides, we have that

$$s\tilde{\pi}(s) - \tilde{\pi}(0) = \tilde{\pi}(s)Q.$$

Equivalently, we have the following expression for $\tilde{\pi}(s)$:

$$\tilde{\pi}(s) = -\tilde{\pi}(0)[Q - sI]^{-1}.$$

These constitute a *structured* system of linear equations. Our goal is to efficiently solve such system of equations for $\bar{\pi}(s)$ and compute the inverse Laplace transform of $\bar{\pi}(s)$ to arrive at the time dependent (transient) PMF of CTMC.

Lemma 2: For a positive recurrent (recurrent non-null) CTMC, in the Region of Convergence (ROC) (of Laplace transform) the sub-matrices on the diagonal of $(Q - sI)$ are non-singular.

Proof: As in the equilibrium case, such matrices are all strictly diagonally dominant and hence are all non-singular. □

Thus, as in the case of computation of equilibrium PMF, $\bar{\pi}(s)$ can be determined efficiently for the values of s lying in the Region of Convergence. Detailed duplication of equations is avoided for brevity.

5 Conclusions

In this research paper, efficient algorithms for computing the equilibrium and transient probability distribution of an arbitrary finite state space CTMC are discussed. The algorithms effectively solve a structured system of linear equations efficiently. It might be interesting to apply the proposed method to solving system of linear equations, where the coefficient matrix has the structure similar to a generator matrix (i.e. structured diagonally dominant matrix), for instance, the generator matrix has Toeplitz structure in some applications. This idea, however, is left for future research.

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