

Inherent Numerical Instability in Computing Invariant Measures of Markov Chains

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How to cite this paper: Baumann, H. and Hanschke, T. (2017) Inherent Numerical Instability in Computing Invariant Measures of Markov Chains. *Applied Mathematics*, 8, 1367-1385.

<https://doi.org/10.4236/am.2017.89101>

Received: August 14, 2017

Accepted: September 27, 2017

Published: September 30, 2017

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Abstract

Invariant measures of Markov chains in discrete or continuous time with a countable set of states are characterized by its steady state recurrence relations. Exemplarily, we consider transition matrices and Q-matrices with upper bandwidth n and lower bandwidth l where the invariant measures satisfy an $(n + 1)$ -order linear difference equation. Markov chains of this type arise from applications to queueing problems and population dynamics. It is the purpose of this paper to point out that the forward use of this difference equation is subject to some hitherto unobserved aspects. By means of the concept of generalized continued fractions (GCFs), we prove that each invariant measure is a dominated solution of the difference equation such that forward computation becomes numerically unstable. Furthermore, the GCF-based approach provides a decoupled recursion in which the phenomenon of numerical instability does not appear. The procedure results in an iteration scheme for successively computing approximants of the desired invariant measure depending on some truncation level N . Increasing N leads to the desired solution. A comparison study of forward computation and the GCF-based approach is given for Q-matrices with upper bandwidth l and 2 .

Keywords

Invariant Measures of Markov Chains, Inherent Numerical Instability of Linear Difference Equations, Generalized Continued Fractions, Convergence Criteria for Generalized Continued Fractions, Truncation Procedures for Infinite Matrices

1. Introduction

This paper is dedicated to discrete-time Markov chains $X = (X_k)_{k \geq 0}$ with a countably infinite set of states (labelled as $0, 1, 2, \dots$) and a stationary one-step

transition matrix $P = (P_{ik})_{0 \leq i, k < \infty}$ of the form

$$P = \begin{bmatrix} P_{00} & P_{01} & P_{02} & \cdots & P_{0n} & O & O & \cdots & \cdots \\ P_{10} & P_{11} & P_{12} & \cdots & P_{1n} & P_{1,n+1} & O & \cdots & \cdots \\ O & P_{21} & P_{22} & \cdots & P_{2n} & P_{2,n+1} & P_{2,n+2} & O & \cdots \\ O & O & P_{32} & \cdots & P_{3n} & P_{3,n+1} & P_{3,n+2} & P_{3,n+3} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad (1)$$

with $n \geq 1$ and $P_{k,k+n} \neq 0$ for at least one $k \in \mathbb{N}_0 = \{0, 1, 2, \dots\}$. In addition we assume that X is irreducible and recurrent. Notice that the irreducibility of X implies

$$P_{k,k-1} \neq 0 \text{ for } k = 1, 2, \dots \quad (2)$$

For a recurrent irreducible Markov chain, the system

$$\begin{cases} x_k = \sum_{i=0}^{\infty} x_i P_{ik} & (k = 0, 1, 2, \dots) \\ x_0 = 1, x_k \geq 0 & (k = 1, 2, \dots) \end{cases} \quad (3)$$

has a unique solution which is strictly positive, see Karlin and Taylor ([1], chapter 11). Every constant positive multiple of $x = (x_0, x_1, \dots)$ is called an invariant measure of X .

Substituting (1) into (3) and rearranging yields the $(n + 1)$ th-order homogeneous linear recurrence relation

$$P_{k+n+1,k+n} x_{k+n+1} + (P_{k+n,k+n} - 1) x_{k+n} + \dots + P_{k,k+n} x_k = 0 \quad (k = 0, 1, 2, \dots) \quad (4)$$

coupled to the side conditions

$$\begin{cases} P_{00} x_0 + P_{10} x_1 = x_0 \\ P_{01} x_0 + P_{11} x_1 + P_{21} x_2 = x_1 \\ \vdots \\ P_{0,n-1} x_0 + P_{1,n-1} x_1 + \dots + P_{n,n-1} x_n = x_{n-1} \end{cases} \quad (5)$$

From the theory of linear difference equations (see Miller [2]) it is known that there exist $n + 1$ linearly independent functions $x^{(0)}, x^{(1)}, \dots, x^{(n)}$ defined on \mathbb{N}_0 which take on prescribed values at $k = 0, 1, \dots, n$ and satisfy the homogeneous recurrence relation (4) for all $k \geq 0$.

Since $P_{k+n+1,k+n} \neq 0$ for all k the desired solution $(x_k)_{k=0}^{\infty}$ is uniquely determined by its initial values x_0, x_1, \dots, x_n and (5). An application of the recurrence relation (4) then should directly lead to the desired solution x . But unfortunately forward computation of x by means of the homogeneous equation (4) is not a meaningful procedure. In the sequel it is shown that the solution space S of the recurrence relation (4) is the direct sum

$$S = S_1 \oplus S_2$$

of two subspaces S_1 and S_2 with the property, that every solution $y \in S_2$ dominates over every solution $x \in S_1$, i.e.

$$\lim_{k \rightarrow \infty} \frac{x_k}{y_k} = 0.$$

In addition, we have $\dim S_1 = n$, $\dim S_2 = 1$ and $x \in S_1$.

As pointed out by Cash [3], Gautschi [4] [5], Lozier [6] and Mattheij [7], forward computation of a dominated solution becomes numerically unstable. To avoid numerical instability, it is therefore necessary to construct a decoupled recursion in which the dominant solution $y \in S_2$ does not appear. In the sequel, it is shown that with each transition matrix P of the form (1) one can associate a set of so-called generalized continued fractions (GCFs) being convergent if the underlying Markov chain is irreducible and recurrent. It turns out that the limits of these fractions coincide with the coefficients of the desired decoupled recursion.

The phenomenon of inherent instability has been first recognized in connection with the computation of higher transcendental functions such as Bessel and associated Legendre functions (see Gautschi [4] and Wimp [8]). Our experience seems to indicate that also most of the recurrence relations arising from stochastic modelling are subject to numerical instability and require special attention. Transition matrices and Q -matrices with lower bandwidth n and upper bandwidth 1 have been discussed in [9].

Remark. Most of our considerations concerning the computation of invariant measures of Markov chains may be extended to more general infinite systems of equations. In Section 3, we will point out the properties of invariant measures which we explicitly used.

2. Generalized Continued Fractions and Linear Difference Equations

This chapter deals with the computation of dominated solutions of homogeneous linear difference equations by means of generalized continued fractions (GCFs). The theory of GCFs was initiated by Jacobi [10] and Perron [11] [12] and played a leading role in different areas of mathematics, especially in number theory, ergodic theory, linear difference equations and Padé approximations.

Definition 1. A generalized continued fraction (GCF) of dimension n is an $(n+1)$ -tuple $(a^{(1)}, \dots, a^{(n)}, b)$ of real-valued sequences and a convergence structure as follows. Let $A^{(1)}, \dots, A^{(n)}, B$ be the principal solutions of the corresponding homogeneous linear difference equation

$$x_{k+n+1} = b_k x_{k+n} + a_k^{(n)} x_{k+n-1} + \dots + a_k^{(1)} x_k \quad (k = 0, 1, 2, \dots) \quad (6)$$

satisfying

$$\begin{cases} A_j^{(i)} = \delta_{i,j+1} = \begin{cases} 1 & \text{for } i = j+1 \\ 0 & \text{for } i \neq j+1 \end{cases} \quad (i = 1, \dots, n; j = 0, \dots, n) \\ B_j = 0 \text{ for } j = 0, \dots, n-1 \text{ and } B_n = 1. \end{cases} \quad (7)$$

The GCF is said to converge iff all the limits

$$\xi^{(i)} = \lim_{k \rightarrow \infty} A_k^{(i)} / B_k \quad (i = 1, \dots, n) \quad (8)$$

do exist.

Convergence of a GCF is indicated by the notation

$$\begin{bmatrix} \xi^{(1)} \\ \vdots \\ \xi^{(n)} \end{bmatrix} \stackrel{k}{=} \begin{bmatrix} a_0^{(1)} & a_1^{(1)} & a_2^{(1)} & \cdots \\ \vdots & \vdots & \vdots & \\ a_0^{(n)} & a_1^{(n)} & a_2^{(n)} & \cdots \\ b_0 & b_1 & b_2 & \cdots \end{bmatrix}.$$

Terminating a GCF after the N -th column we get the so-called N -th approximants

$$\begin{bmatrix} \frac{A_{N+n+1}^{(1)}}{B_{N+n+1}} \\ \vdots \\ \frac{A_{N+n+1}^{(n)}}{B_{N+n+1}} \end{bmatrix} = \begin{bmatrix} a_0^{(1)} & a_1^{(1)} & \cdots & a_N^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ a_0^{(n)} & a_1^{(n)} & \cdots & a_N^{(n)} \\ b_0 & b_1 & \cdots & b_N \end{bmatrix}.$$

The term ‘‘GCF’’ becomes obvious if forward computation of the N -th approximant of a GCF is replaced by the equivalent backward algorithm. It is known that the recurrence relation (6) can be converted into a first order vector recursion of the form

$$u_{k+1} = W_k u_k \quad (k = 0, 1, 2, \dots) \tag{9}$$

by putting

$$u_k = \begin{bmatrix} x_k \\ x_{k+1} \\ \vdots \\ x_{k+n-1} \\ x_{k+n} \end{bmatrix} \text{ and } W_k = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \cdots & 0 & 1 \\ a_k^{(1)} & a_k^{(2)} & \cdots & \cdots & a_k^{(n)} & b_k \end{bmatrix} \quad (k = 0, 1, 2, \dots).$$

Comparing (6) and (9) it is seen, that the numerators $A_{N+n+1}^{(1)}, \dots, A_{N+n+1}^{(n)}$ and the denominators B_{N+n+1} of the GCF appear in the last row of the matrix

$$W_N W_{N-1} \cdots W_0.$$

Consider now the backward recurrence scheme

$${}^{(N)}v_k = {}^{(N)}v_{k+1} W_k \quad (k = N, N-1, \dots, 0) \tag{10}$$

with initial vector ${}^{(N)}v_{N+1} = (0, \dots, 0, 1)$. Then

$${}^{(N)}v_0 = {}^{(N)}v_{N+1} W_N W_{N-1} \cdots W_0 = (A_{N+n+1}^{(1)}, \dots, A_{N+n+1}^{(n)}, B_{N+n+1}).$$

Writing (10) in expanded form and inserting the structure of W_k , we get

$$\begin{aligned} {}^{(N)}v_k^{(1)} &= {}^{(N)}v_{k+1}^{(n+1)} a_k^{(1)} \quad (k = N, N-1, \dots, 0), \\ {}^{(N)}v_k^{(i)} &= {}^{(N)}v_{k+1}^{(i-1)} + {}^{(N)}v_{k+1}^{(n+1)} a_k^{(i)} \quad (i = 2, \dots, n, k = N, N-1, \dots, 0), \\ {}^{(N)}v_k^{(n+1)} &= {}^{(N)}v_{k+1}^{(n)} + {}^{(N)}v_{k+1}^{(n+1)} b_k \quad (k = N, N-1, \dots, 0) \end{aligned}$$

or, equivalently

$$\begin{cases} \binom{(N)}{r_k^{(1)}} := \frac{\binom{(N)}{v_k^{(1)}}}{\binom{(N)}{v_k^{(n+1)}}} = \frac{a_k^{(1)}}{b_k + \binom{(N)}{r_{k+1}^{(n)}}} & (k = N, N-1, \dots, 0) \\ \binom{(N)}{r_k^{(i)}} := \frac{\binom{(N)}{v_k^{(i)}}}{\binom{(N)}{v_k^{(n+1)}}} = \frac{a_k^{(i)} + \binom{(N)}{r_{k+1}^{(i-1)}}}{b_k + \binom{(N)}{r_{k+1}^{(n)}}} & (i = 2, \dots, n; k = N, N-1, \dots, 0) \end{cases} \quad (11)$$

with initial values $\binom{(N)}{r_{N+1}^{(i)}} = 0$ for $i = 1, \dots, n$. Hence

$$\frac{A_{N+n+1}^{(i)}}{B_{N+n+1}} = \binom{(N)}{r_0^{(i)}} \quad (i = 1, \dots, n)$$

and

$$\xi^{(i)} = \lim_{N \rightarrow \infty} \binom{(N)}{r_0^{(i)}} \quad (i = 1, \dots, n). \quad (12)$$

Alternative procedures for computing GCFs are described in [13].

The relations between GCFs and linear difference equations have been first recognized by Perron [14]. Perron's results were generalized by Van der Cruyssen [13], Hanschke [15] [16] and Levrie and Bultheel [17]. The following theorem is due to Van der Cruyssen [13].

Theorem 1. A GCF $(a^{(1)}, \dots, a^{(n)}, b)$ converges iff there are $n+1$ linearly independent solutions $x^{(1)}, \dots, x^{(n)}, y$ of the recurrence relation (6) satisfying

$$\lim_{k \rightarrow \infty} \frac{x_k^{(i)}}{y_k} = 0 \quad (i = 1, \dots, n) \quad (13)$$

and

$$\begin{vmatrix} x_0^{(1)} & \dots & x_{n-1}^{(1)} \\ \vdots & & \vdots \\ x_0^{(n)} & \dots & x_{n-1}^{(n)} \end{vmatrix} \neq 0. \quad (14)$$

As pointed out by Gautschi [4] [5] and Van der Cruyssen [13], forward computation of a solution $x \in \text{span}(x^{(1)}, \dots, x^{(n)})$ is numerically unstable. Van der Cruyssen [13] establishes that if the limits

$$\begin{bmatrix} \xi_l^{(1)} \\ \vdots \\ \xi_l^{(n)} \end{bmatrix} = \begin{bmatrix} a_l^{(1)} & a_{l+1}^{(1)} & a_{l+2}^{(1)} & \dots \\ \vdots & \vdots & \vdots & \\ a_l^{(n)} & a_{l+1}^{(n)} & a_{l+2}^{(n)} & \dots \\ b_l & b_{l+1} & b_{l+2} & \dots \end{bmatrix} \quad (15)$$

exist for all $l \geq 0$, then $x \in \text{span}(x^{(1)}, \dots, x^{(n)})$ iff

$$x_{l+n} = -\xi_l^{(n)} x_{l+n-1} - \dots - \xi_l^{(1)} x_l \quad (l = 0, 1, 2, \dots). \quad (16)$$

Combining (11), (12) and (16), one obtains an efficient algorithm (which we will refer to as *Van der Cruyssen's algorithm*) for approximating the first $L+1$ components x_0, \dots, x_L of an element $x \in \text{span}(x^{(1)}, \dots, x^{(n)})$ with prescribed values x_0, \dots, x_{n-1} :

Step 1: Select $N > L - n$ and define $\binom{(N)}{r_l^{(i)}}$ for $i = 1, \dots, n; l = 0, 1, \dots, N+1$ by

$$\begin{aligned}
 &({}^{(N)}r_{N+1}^{(1)} = \dots = {}^{(N)}r_{N+1}^{(n)} = 0, \\
 &({}^{(N)}r_l^{(1)} = \frac{a_l^{(1)}}{b_l + ({}^{(N)}r_{l+1}^{(n)})} \quad (l = N, N-1, \dots, 0), \\
 &({}^{(N)}r_l^{(i)} = \frac{a_l^{(i)} + ({}^{(N)}r_{l+1}^{(i-1)})}{b_l + ({}^{(N)}r_{l+1}^{(n)})} \quad (i = 2, \dots, n; l = N, N-1, \dots, 0).
 \end{aligned}$$

Step 2: Set $({}^{(N)}x_0 = x_0, \dots, ({}^{(N)}x_{n-1} = x_{n-1})$ and

$$({}^{(N)}x_{l+n} = -({}^{(N)}r_l^{(n)} ({}^{(N)}x_{l+n-1} - \dots - ({}^{(N)}r_l^{(1)} ({}^{(N)}x_l$$

for $l = 0, 1, \dots, L-n$.

Step 3: Increase N until the accuracy of the iterates is within prescribed limits.

For any l , the vector $(({}^{(N)}r_l^{(1)}, \dots, ({}^{(N)}r_l^{(n)})^T$ is an approximant of a GCF. Hence, convergence of the algorithm is related to convergence of GCFs. For the latter, we cite two helpful results.

Theorem 2. (Levrie [18], Perron [12]). *The GCF*

$$\begin{bmatrix} a_0^{(1)} & a_1^{(1)} & a_2^{(1)} & \dots \\ \vdots & \vdots & \vdots & \\ a_0^{(n)} & a_1^{(n)} & a_2^{(n)} & \dots \\ b_0 & b_1 & b_2 & \dots \end{bmatrix}$$

converges if it satisfies the so-called dominance condition, *i.e.*

$$|a_k^{(1)}| + |a_k^{(2)}| + \dots + |a_k^{(n)}| + 1 \leq |b_k| \quad \text{for all } k \geq 0.$$

Theorem 3. (De Bruin [19], Perron [12]). Consider a GCF of the form (8) with v th approximant numerators $A_{v+n+1}^{(i)} (i = 1, \dots, n)$ and denominators B_{v+n+1} and the GCF given by

$$\begin{bmatrix} a_0^{(1)} \rho_0 \rho_{-1} \dots \rho_{-n} & a_1^{(1)} \rho_1 \rho_0 \dots \rho_{1-n} & \dots & a_v^{(1)} \rho_v \rho_{v-1} \dots \rho_{v-n} \dots \\ a_0^{(2)} \rho_0 \rho_{-1} \dots \rho_{1-n} & a_1^{(2)} \rho_1 \rho_0 \dots \rho_{2-n} & \dots & a_v^{(2)} \rho_v \rho_{v-1} \dots \rho_{v-n+1} \\ \vdots & \vdots & & \vdots \\ a_0^{(n)} \rho_0 \rho_{-1} & a_1^{(n)} \rho_1 \rho_0 & & a_v^{(n)} \rho_v \rho_{v-1} \\ b_0 \rho_0 & b_1 \rho_1 & & b_v \rho_v \end{bmatrix} \quad (17)$$

with v th numerators $\tilde{A}_{v+n+1}^{(i)} (i = 1, \dots, n)$ and denominators \tilde{B}_{v+n+1} where the real numbers $\rho_{-n}, \rho_{-n+1}, \dots, \rho_0, \rho_1, \dots$ are all different from zero. Then

$$\left. \begin{aligned} \tilde{A}_{v+n+1}^{(i)} &= \rho_v \rho_{v-1} \dots \rho_1 \rho_0 \dots \rho_{-n+i-1} A_{v+n+1}^{(i)} \quad (i = 1, \dots, n) \\ \tilde{B}_{v+n+1} &= \rho_v \rho_{v-1} \dots \rho_0 B_{v+n+1} \end{aligned} \right\} v \in \mathbb{N}_0$$

In other words, if one of these two GCFs converges so does the other.

Notice that the GCF (17) may be interpreted as an equivalence transformation of the GCF (12).

3. Main Results

To make (4) congruent with (6) we put

$$a_k^{(i)} = -\frac{P_{k+i-1,k+n}}{P_{k+n+1,k+n}} \quad (i = 1, \dots, n, k = 0, 1, 2, \dots), \tag{18}$$

$$b_k = -\frac{P_{k+n,k+n} - 1}{P_{k+n+1,k+n}} \quad (k = 0, 1, 2, \dots). \tag{19}$$

Theorem 4. Let $a_k^{(i)}, b_k$ be defined as in (18) and (19). The limits

$$\begin{bmatrix} \xi_l^{(1)} \\ \vdots \\ \xi_l^{(n)} \end{bmatrix} = \begin{bmatrix} a_l^{(1)} & a_{l+1}^{(1)} & a_{l+2}^{(1)} & \cdots \\ \vdots & \vdots & \vdots & \\ a_l^{(n)} & a_{l+1}^{(n)} & a_{l+2}^{(n)} & \cdots \\ b_l & b_{l+1} & b_{l+2} & \cdots \end{bmatrix} \tag{20}$$

exist for all $l \geq 0$ if the corresponding Markov chain is irreducible and recurrent. In case of convergence the invariant measure is a dominated solution of (6) and satisfies the decoupled recursion

$$x_{l+n} = -\xi_l^{(n)} x_{l+n-1} - \dots - \xi_l^{(1)} x_l \quad (l = 0, 1, 2, \dots). \tag{21}$$

Proof. Denote by ${}_{(N)}P = (P_{ik})_{0 \leq i, k \leq N}$ the $(N+1) \times (N+1)$ northwest corner truncation of P . Since P is assumed to be irreducible and recurrent we conclude from Seneta [20] [21] [22] that the finite system

$${}_{(N)}h \left({}_{(N)}I - {}_{(N)}P \right) = e_0 \tag{22}$$

where ${}_{(N)}I$ is the unit matrix and ${}_{(N)}e_0$ is the vector with unity in the first position and zeros elsewhere has a unique solution ${}_{(N)}h = ({}_{(N)}h_0, {}_{(N)}h_1, \dots, {}_{(N)}h_N)$ satisfying

$$\lim_{N \rightarrow \infty} \frac{{}_{(N)}h_k}{{}_{(N)}h_0} = \frac{x_k}{x_0} \quad (k = 0, 1, 2, \dots).$$

The vector ${}_{(N)}h$ satisfies the homogeneous linear difference Equation (6) for $k = 0, 1, \dots, N - n$ and is subject to the boundary conditions

$$\left. \begin{aligned} (1 - P_{00}) {}_{(N)}h_0 - P_{10} {}_{(N)}h_1 &= 1 \\ -P_{01} {}_{(N)}h_0 + (1 - P_{11}) {}_{(N)}h_1 - P_{21} {}_{(N)}h_2 &= 0 \\ &\vdots \\ -P_{0,n-1} {}_{(N)}h_0 - P_{1,n-1} {}_{(N)}h_1 - \dots - P_{n,n-1} {}_{(N)}h_n &= 0 \end{aligned} \right\} \tag{23}$$

and

$${}_{(N)}h_{N+1} = 0. \tag{24}$$

Notice that the numerators $A_l^{(1)}, \dots, A_l^{(n)}$ and the denominators B_l of the GCF (20) satisfy

$$x_{k+n+1} = b_{k+l} x_{k+n} + a_{k+l}^{(n)} x_{k+n-1} + \dots + a_{k+l}^{(1)} x_k \quad (k = 0, 1, 2, \dots) \tag{25}$$

and build up a fundamental system of solutions to Equation (6) for $k \geq l$.

Hence any solution of the recurrence relation (6) can be expressed in terms of these functions. In view of their initial values

$$\begin{cases} A_{l,j}^{(i)} = \delta_{i,j+1} = \begin{cases} 1 & \text{for } i = j + 1 \\ 0 & \text{for } i \neq j + 1 \end{cases} \quad (i = 1, \dots, n; j = 0, \dots, n) \\ B_{l,j} = 0 \quad \text{for } j = 0, \dots, n - 1 \text{ and } B_{l,l+n} = 1; \end{cases} \quad (26)$$

we get

$${}_{(N)}h_k = {}_{(N)}h_l A_{l,k-l}^{(1)} + \dots + {}_{(N)}h_{l+n-1} A_{l,k-l}^{(n)} + {}_{(N)}h_{l+n} B_{l,k-l} \quad (k = l, l + 1, \dots). \quad (27)$$

Choosing $k = N + 1$ and utilizing (24) equation (27) reduces to

$${}_{(N)}h_{l+n} B_{l,N-l+1} = -{}_{(N)}h_l A_{l,N-l+1}^{(1)} - \dots - {}_{(N)}h_{l+n-1} A_{l,N-l+1}^{(n)}. \quad (28)$$

Dividing both sides of (28) by $B_{l,N-l+1}$ and ${}_{(N)}h_0$ we formally arrive at

$$\frac{{}_{(N)}h_{l+n}}{{}_{(N)}h_0} = -\frac{{}_{(N)}h_l A_{l,N-l+1}^{(1)}}{{}_{(N)}h_0 B_{l,N-l+1}} - \dots - \frac{{}_{(N)}h_{l+n-1} A_{l,N-l+1}^{(n)}}{{}_{(N)}h_0 B_{l,N-l+1}}. \quad (29)$$

Passing to the limit $N \rightarrow \infty$ we get the decoupled recursion (21) provided that the limits $\lim_{N \rightarrow \infty} A_{l,N-l+1}^{(i)} / B_{l,N-l+1}$ do exist for $i = 0, 1, \dots, n$.

To prove our assertion we utilize that the invariant measure $(x_k)_{k \geq 0}$ of the irreducible and recurrent Markov chain (1) is strictly positive and satisfies the recurrence relation (4) which can be rewritten as

$$\begin{aligned} & \frac{P_{k,k+n} \cdot x_k}{P_{k+n+1,k+n} \cdot x_{k+n+1}} + \frac{P_{k+1,k+n} \cdot x_{k+1}}{P_{k+n+1,k+n} \cdot x_{k+n+1}} + \dots + \frac{P_{k+n-1,k+n} \cdot x_{k+n-1}}{P_{k+n+1,k+n} \cdot x_{k+n+1}} + 1 \\ &= \frac{(1 - P_{k+n,k+n}) x_{k+n}}{P_{k+n+1,k+n} \cdot x_{k+n+1}} \quad (k = 0, 1, 2, \dots). \end{aligned} \quad (30)$$

Define $\rho_k = \frac{x_{k+n}}{x_{k+n+1}}$ for $k = 0, 1, 2, \dots$ Then (30) becomes equivalent to

$$\begin{aligned} & \left| a_k^{(1)} \rho_k \rho_{k-1} \dots \rho_{k-n} \right| + \left| a_k^{(2)} \rho_k \rho_{k-1} \dots \rho_{k-n+1} \right| \\ & + \dots + \left| a_k^{(n)} \rho_k \rho_{k-1} \right| + 1 = \left| b_k \rho_k \right| \quad (k = 0, 1, 2, \dots) \end{aligned}$$

implying that the GCFs

$$\begin{bmatrix} a_l^{(1)} \rho_l \rho_{l-1} \dots \rho_{l-n} & a_{l+1}^{(1)} \rho_{l+1} \rho_l \dots \rho_{l-n+1} & \dots \\ a_l^{(2)} \rho_l \rho_{l-1} \dots \rho_{l-n+1} & a_{l+1}^{(2)} \rho_{l+1} \rho_l \dots \rho_{l-n+2} & \dots \\ \vdots & \vdots & \\ a_l^{(n)} \rho_l \rho_{l-1} & a_{l+1}^{(n)} \rho_{l+1} \rho_l & \dots \\ b_l \rho_l & b_{l+1} \rho_l & \dots \end{bmatrix}$$

converge for all $l \geq 0$ by means of Theorem 2. From Theorem 3, we then conclude that the same is true for the GCFs (8). \square

Theorem 2 says that the numerical calculation of the invariant measures of X

can be reduced to Van der Cruyssen's algorithm with (23) as initial conditions.

Remark. It is important that the statement of Theorem 4 consists of two parts:

- The invariant measure is dominated by other solutions of the difference Equation (4).
- By means of GCFs, we are able to construct a decoupled recursion which is not affected to numerical instability.

Our main goal was the derivation of the first statement. Although the existence of dominating solutions has been pointed out in specific examples (e.g. ([8], p. 167) where the exact solutions of the difference equations are known), to our knowledge, no statement in this generality has been published. Since the desired solution being dominated directly implies numerical instability, the system $x = xP$ should not be solved by forward computation. Note, that up to some slight modifications concerning the boundary conditions, the truncated system (22) yields the same difference Equation (4) for $k = 0, 1, \dots, N - n - 1$. Thus, forward computation could be applied to (22), too, but at least for large N , the result of numerical instability and hence, the recommendation not to use forward computation, holds for (22) as well.

The observation of inherent numerical instability of (4) is essential since the transition structure under consideration arises in many practical applications, e.g. state-dependent queueing systems with bulk arrivals, and it is also valid in a more general context, e.g. as an approximation to state-dependent variants of the traditional $G/M/1$ queueing model.

Basically, we have exploited that the solutions of the truncated system (22) converge to invariant measures as $N \rightarrow \infty$. For Markov chains with a general transition structure, there is no way of solving $x = xP$ directly (in particular, forward computation cannot be applied if $P_{kl} > 0$ for some $k < l - 1$). In this situation, Seneta [20] [21] [22] as well as Golub and Seneta [23] already recommended to use the convergence of the solutions of the truncated system (22) to the invariant measure for numerical issues. Furthermore, Seneta [22] discussed numerical aspects (in terms of the condition number) of the finite system (22) and stated numerical stability of Gaussian elimination or LU decomposition. The above comment concerning forward computation as a solution method for (22) emphasizes on the fact that it is important to solve this finite system in an appropriate way. The GCF-based algorithm can be interpreted as a combination of building up the truncated system (22), and then applying a modification of Gaussian elimination procedure. Therefore, it follows both steps recommended in the literature cited above and represents the complete procedure in a combined mathematical form, which is interesting from a structural point of view.

4. Continuous-Time Markov Chains

The results of the preceding chapter can easily be extended to continuous-time Markov chains $Y = (Y_t)_{t \geq 0}$ generated by a conservative, irreducible and regular

Q-matrix of the form

$$Q = \begin{bmatrix} q_{00} & q_{01} & q_{02} & \cdots & q_{0n} & O & O & \cdots & \cdots \\ q_{10} & q_{11} & q_{12} & \cdots & q_{1n} & q_{1,n+1} & O & \cdots & \cdots \\ O & q_{21} & q_{22} & \cdots & q_{2n} & q_{2,n+1} & q_{2,n+2} & O & \cdots \\ O & O & q_{32} & \cdots & q_{3n} & q_{3,n+1} & q_{3,n+2} & q_{3,n+3} & \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad (31)$$

where $n \geq 1$ and $q_{k,k+n} \neq 0$ for at least one $k \in \mathbb{N}_0$. Notice that the irreducibility of Y implies

$$q_{k,k-1} \neq 0 \text{ for } k = 1, 2, \dots$$

If Y is positive recurrent, the limits

$$\pi_k = \lim_{t \rightarrow \infty} P(Y_t = k | Y_0 = i) \quad (k = 0, 1, 2, \dots)$$

exist independently of the initial state and build up a probability distribution which is strictly positive. For the construction of a continuous-time Markov process from its infinitesimal properties the reader is referred to Reuter [24] and Kendall and Reuter [25]. Now let ${}_{(N)}Q$ be the $(N+1) \times (N+1)$ northwest corner truncation of Q . If Y is regular and positive recurrent, then the finite system

$${}_{(N)}z {}_{(N)}Q = {}_{(N)}e_0 \quad (32)$$

has a unique solution ${}_{(N)}z = ({}_{(N)}z_0, {}_{(N)}z_1, \dots, {}_{(N)}z_N)$ satisfying

$$\lim_{N \rightarrow \infty} \frac{{}_{(N)}z_k}{{}_{(N)}z_0} = \frac{\pi_k}{\pi_0} \quad (k = 0, 1, 2, \dots),$$

see Tweedie [26]. Now let

$$c_k^{(i)} = -\frac{q_{k+i-1,k+n}}{q_{k+n+1,k+n}} \quad (i = 1, \dots, n, \quad k = 0, 1, 2, \dots), \quad (33)$$

$$d_k = -\frac{q_{k+n,k+n}}{q_{k+n+1,k+n}} \quad (k = 0, 1, 2, \dots). \quad (34)$$

By substituting (31) into (32) it is seen that ${}_{(N)}z$ satisfies the $(n+1)$ th order homogeneous linear difference equation

$$\pi_{k+n+1} = d_k \pi_{k+n} + c_k^{(n)} \pi_{k+n-1} + \dots + c_k^{(1)} \pi_k \quad (k = 0, 1, 2, \dots) \quad (35)$$

for $k = 0, 1, \dots, N-n$ and the boundary conditions

$$\left. \begin{aligned} q_{00} {}_{(N)}z_0 + q_{10} {}_{(N)}z_1 &= 1 \\ q_{01} {}_{(N)}z_0 + q_{11} {}_{(N)}z_1 + q_{21} {}_{(N)}z_2 &= 0 \\ &\vdots \\ q_{0,n-1} {}_{(N)}z_0 + q_{1,n-1} {}_{(N)}z_1 + \dots + q_{n,n-1} {}_{(N)}z_n &= 0 \end{aligned} \right\} \quad (36)$$

$${}_{(N)}z_{N+1} = 0. \quad (37)$$

By replacing (33) with (18) and (34) with (19), it is readily seen that the scheme (35)-(37) formally coincides with that of the discrete time case. Hence (26)-(29) also hold for ${}_{(N)}z_t$. To prove convergence of the associated GCFs

$$\begin{bmatrix} \Lambda_l^{(1)} \\ \vdots \\ \Lambda_l^{(n)} \end{bmatrix} = \begin{bmatrix} c_l^{(1)} & c_{l+1}^{(1)} & c_{l+2}^{(1)} & \cdots \\ \vdots & \vdots & \vdots & \\ c_l^{(n)} & c_{l+1}^{(n)} & c_{l+2}^{(n)} & \cdots \\ d_l & d_{l+1} & d_{l+2} & \cdots \end{bmatrix} \quad (l = 0, 1, 2, \dots) \quad (38)$$

we use the same arguments as in the proof of Theorem 4. Notice that $(\pi_k)_{k=0}^\infty$ satisfies (35). Rearranging yields

$$-c_k^{(1)} \frac{\pi_k}{\pi_{k+n+1}} - \dots - c_k^{(n)} \frac{\pi_{k+n-1}}{\pi_{k+n+1}} + 1 = d_k \frac{\pi_{k+n}}{\pi_{k+n+1}} \quad (k = 0, 1, 2, \dots). \quad (39)$$

Define $\gamma_k = \frac{\pi_{k+n}}{\pi_{k+n+1}}$ for $k = 0, 1, 2, \dots$. Since $-c_k^{(i)} > 0$ for $i = 1, \dots, n, k \geq 0$ and $d_k > 0$ for $k \geq 0$, (39) is equivalent to

$$\begin{aligned} & \left| c_k^{(1)} \gamma_k \gamma_{k-1} \cdots \gamma_{k-n} \right| + \left| c_k^{(2)} \gamma_k \gamma_{k-1} \cdots \gamma_{k-n+1} \right| + \dots + \left| c_k^{(n)} \gamma_k \gamma_{k-1} \right| + 1 \\ & = \left| d_k \gamma_k \right| \quad (k = 0, 1, 2, \dots). \end{aligned}$$

By Theorem 3, the GCF

$$\begin{bmatrix} c_l^{(1)} \gamma_l \gamma_{l-1} \cdots \gamma_{l-n} & c_{l+1}^{(1)} \gamma_{l+1} \gamma_l \cdots \gamma_{l-n+1} & \cdots \\ c_l^{(2)} \gamma_l \gamma_{l-1} \cdots \gamma_{l-n+1} & c_{l+1}^{(2)} \gamma_{l+1} \gamma_l \cdots \gamma_{l-n+2} & \cdots \\ \vdots & \vdots & \\ c_l^{(n)} \gamma_l \gamma_{l-1} & c_{l+1}^{(n)} \gamma_{l+1} \gamma_l & \cdots \\ d_l \gamma_l & d_{l+1} \gamma_l & \cdots \end{bmatrix}$$

then converges for all $l \geq 0$. Hence the same is true for the GCFs (38). Summarizing we arrive at the following theorem.

Theorem 5. Let $c_k^{(i)}, d_k$ be defined as in (33) and (34), respectively. The limits (38) exist for all $l \geq 0$ if the corresponding Markov process is irreducible, regular and positive recurrent. In case of convergence the limiting distribution $(\pi_k)_{k=0}^\infty$ is a dominated solution of (35) and satisfies the decoupled recursion.

$$\pi_{l+n} = -\Lambda_l^{(n)} \pi_{l+n-1} - \dots - \Lambda_l^{(1)} \pi_l \quad (l = 0, 1, 2, \dots). \quad (40)$$

For executing (40), we make use of Van der Cruyssen’s algorithm with (36) as initial conditions. The resulting sequence $\left(\binom{(N)}{(N)} z_k \right)_{k=0}^N$ can be normalized such that $\sum_{k=0}^N \binom{(N)}{(N)} z_k = 1$.

Remark. As for discrete-time Markov chains, the key statement of Theorem 5 is that the invariant measure is a dominated solution of the difference equation (35). Again, the GCFs additionally combine the two-step method consisting of considering the truncated system (32) and applying Gaussian elimination or LU decomposition.

5. Numerical Examples

As an example we consider the continuous-time Markov chain $Y = (Y_t)_{t \geq 0}$ generated by the Q-matrix $Q = (q_{ij})_{0 \leq i, k < \infty}$, where

$$q_{ik} = \begin{cases} \frac{a_0 a_1}{\gamma^i} & k = i - 1, i \geq 1 \\ \frac{a_1 - a_0 - 1}{\gamma^i}, & k = i + 1 \\ \frac{1}{\gamma^i}, & k = i + 2 \\ -\frac{a_1 - a_0}{\gamma^i}, & k = i = 0 \\ -\frac{a_0 a_1 + a_1 - a_0}{\gamma^i}, & k = i \geq 1 \\ 0, & \text{elsewhere} \end{cases} \quad (41)$$

with parameters $a_0 > \gamma > 1$ and $a_1 \geq a_0 + 1$. Such a Markov chain may be interpreted as a model for a single-server queueing system with state-dependent arrival and service rates, and with customers arriving in groups of size 1 or 2.

It is easy to check that Q is irreducible. To prove that Y is regular and positive recurrent we make use of Tweedie's [27] criterion. The condition is to find some $\varepsilon > 0$ and a non-negative sequence $z = (z_0, z_1, \dots)$ satisfying $z_i \rightarrow \infty$ as $i \rightarrow \infty$ and

$$\sum_{k=0}^{\infty} q_{ik} z_k \leq -\varepsilon \quad (42)$$

for almost all i . By substituting (41) into (42) we get

$$\frac{1}{\gamma^i} z_{i+2} + \frac{a_1 - a_0 - 1}{\gamma^i} z_{i+1} - \frac{a_1 - a_0}{\gamma^i} z_i + \frac{a_0 a_1}{\gamma^i} z_{i-1} \leq -\varepsilon$$

for almost all i . The substitution $z_i = \gamma^i$ for $i = 0, 1, 2, \dots$ implies the condition

$$\frac{(\gamma - 1)(\gamma - a_0)(\gamma + a_1)}{\gamma} \leq -\varepsilon$$

for almost all i which is true because of $a_0 > \gamma > 1$.

Under these conditions there exists a unique invariant measure of Y (up to multiplication by a constant), which satisfies the following set of equations:

$$\frac{a_0 a_1}{\gamma} \pi_1 - (a_1 - a_0) \pi_0 = 0, \quad (43)$$

$$\frac{a_0 a_1}{\gamma^2} \pi_2 - \frac{a_0 a_1 + a_1 - a_0}{\gamma} \pi_1 + (a_1 - a_0 - 1) \pi_0 = 0 \quad (44)$$

and

$$\frac{a_0 a_1}{\gamma^{k+3}} \pi_{k+3} - \frac{a_0 a_1 + a_1 - a_0}{\gamma^{k+2}} \pi_{k+2} + \frac{a_1 - a_0 - 1}{\gamma^{k+1}} \pi_{k+1} + \frac{1}{\gamma^k} \pi_k = 0$$

or, equivalently,

$$a_0 a_1 \pi_{k+3} - (a_0 a_1 + a_1 - a_0) \gamma \pi_{k+2} + (a_1 - a_0 - 1) \gamma^2 \pi_{k+1} + \gamma^3 \pi_k = 0 \quad (45)$$

for $k = 0, 1, 2, \dots$. (45) leads to the recursion

$$\pi_{k+3} = \frac{\gamma(a_0 a_1 + a_1 - a_0)\pi_{k+2} - \gamma^2(a_1 - a_0 - 1)\pi_{k+1} - \gamma^3 \pi_k}{a_0 a_1} \tag{46}$$

which is used for forward computation.

Since (45) is a homogenous linear difference equation with constant coefficients a fundamental set of solutions can easily be derived from the roots of its characteristic equation. A simple manipulation yields the following set of linearly independent solutions:

$$\left(\left(\frac{\gamma}{a_0} \right)^k \right)_{k=0}^{\infty}, \left(\left(-\frac{\gamma}{a_1} \right)^k \right)_{k=0}^{\infty}, (\gamma^k)_{k=0}^{\infty}.$$

The desired invariant measure $(\pi_k)_{k=0}^{\infty}$ of Y with initial value $\pi_0 = 1$ is a linear combination of the first two solutions, that is:

$$\pi_k = \frac{a_1}{a_0 + a_1} \left(\frac{\gamma}{a_0} \right)^k + \frac{a_0}{a_0 + a_1} \left(-\frac{\gamma}{a_1} \right)^k \quad (k = 0, 1, 2, \dots).$$

Therefore, choosing $\gamma > 1$ yields that there is a geometrically increasing solution of (46), which explains why forward computation cannot cope with this problem, whereas the GCF-based algorithm becomes a stable procedure. This effect is reflected in **Table 1** and **Table 2**, where data type double in C++ was used.

Table 1. Numerical values for $\gamma = 3, a_0 = 5, a_1 = 7$.

k	Forward computation	GCF based solution	Exact solution
0	1	1	1
1	0.171429	0.171429	0.171429
2	0.286531	0.286531	0.286531
3	0.0932012	0.0932012	0.0932012
4	0.0896566	0.0896566	0.0896566
5	0.0393357	0.0393357	0.0393357
17	9.85074×10^{-5}	9.85075×10^{-5}	9.85075×10^{-5}
18	5.93420×10^{-5}	5.93424×10^{-5}	5.93424×10^{-5}
19	3.55023×10^{-5}	3.55035×10^{-5}	3.55035×10^{-5}
20	2.13423×10^{-5}	2.13458×10^{-5}	2.13458×10^{-5}
21	1.27782×10^{-5}	1.27888×10^{-5}	1.27888×10^{-5}
22	7.64963×10^{-6}	7.68128×10^{-6}	7.68128×10^{-6}
23	4.51039×10^{-6}	4.60533×10^{-6}	4.60533×10^{-6}
24	2.47987×10^{-6}	2.76467×10^{-6}	2.76467×10^{-6}
25	8.03766×10^{-7}	1.65817×10^{-6}	1.65817×10^{-6}
26	-1.56804×10^{-6}	9.95173×10^{-7}	9.95173×10^{-7}
27	-7.09265×10^{-6}	5.96988×10^{-7}	5.96988×10^{-7}
28	-2.27107×10^{-5}	3.58242×10^{-7}	3.58242×10^{-7}
29	-6.89918×10^{-5}	2.14924×10^{-7}	2.14924×10^{-7}
30	-0.000207491	1.28964×10^{-7}	1.28964×10^{-7}
40	-12.2598	7.79771×10^{-10}	7.79771×10^{-10}
50	-723,927	4.71497×10^{-12}	4.71497×10^{-12}

Table 2. Numerical values for $\gamma = 9, a_0 = 10, a_1 = 12$.

k	Forward computation	GCF based solution	Exact solution
0	1	1	1
1	0.15	0.15	0.15
2	0.6975	0.6975	0.6975
3	0.205875	0.205875	0.205875
4	0.501694	0.501694	0.501694
5	0.21422	0.21422	0.21422
13	0.127849	0.127848	0.127848
14	0.132884	0.132882	0.132882
15	0.106256	0.10623	0.10623
16	0.105863	0.10563	0.10563
17	0.0896527	0.0875497	0.0875497
18	0.10336	0.0844324	0.0844324
19	0.242111	0.0717609	0.0717609
20	1.60091	0.067756	0.067756
21	13.857	0.058602	0.058602
22	124.24	0.0545256	0.0545256
23	1117.72	0.0477352	0.0477352
24	10,059.1	0.0439651	0.0439651
25	90,531.2	0.038816	0.038816

Consider next the M/M/1 queueing system, in which the customers arrive according to a Poisson stream with rate $\lambda > 0$ and in which the successive service times are stochastically independent and exponentially distributed with parameter $\mu > 0$. For this system it is known that the queueing process $L = (L(t))_{t \geq 0}$ which counts the number of customers in line, forms a homogeneous continuous time Markov chain with state space $\mathbb{N}_0 = \{0, 1, 2, \dots\}$ being regular and positive recurrent for $\rho = \frac{\lambda}{\mu} < 1$, see [28]. The model is convenient to get clear about the mechanism of our approach.

The invariant measure $(\pi_k)_{k=0}^\infty$ of L meets the second order linear difference equation

$$\lambda \pi_{k-1} - (\lambda + \mu) \pi_k + \mu \pi_{k+1} = 0 \quad (k = 1, 2, \dots) \tag{47}$$

subject to the side conditions

$$\pi_0 = 1 \text{ and } -\lambda \pi_0 + \mu \pi_1 = 0.$$

In principle, $(\pi_k)_{k=0}^\infty$ could be computed by forward computation, that is

$$\begin{aligned} \pi_0 &= 1, \\ \pi_1 &= \rho \pi_0, \end{aligned}$$

$$\pi_{k+1} = (\rho + 1)\pi_k - \rho\pi_{k-1} \quad (k = 1, 2, \dots),$$

where $\rho = \frac{\lambda}{\mu} < 1$.

A simple induction argument shows that $\pi_k = \rho^k$ for $k = 0, 1, 2, \dots$. Another solution of (47) is given by $\tilde{\pi}_k = 1$ for $k = 0, 1, 2, \dots$, implying that $(\pi_k)_{k=0}^\infty$ becomes a dominated solution of (47), as claimed. Therefore $(\pi_k)_{k=0}^\infty$ can also be characterized by the decoupled recursion (40), *i.e.*

$$\pi_{k+1} = -\Lambda_k^{(1)}\pi_k \quad (k = 0, 1, 2, \dots). \tag{48}$$

Substituting of (48) into (47) leads to

$$\Lambda_{k-1}^{(1)} = -\frac{1}{(1 + \rho^{-1}) + \rho^{-1}\Lambda_k^{(1)}} \quad (k = 1, 2, \dots). \tag{49}$$

By truncating this infinite continued fraction scheme at a certain level $k = N$, we get approximants for the desired coefficients $\Lambda_k^{(1)}$. A numerical example is given in **Table 3**. In this example the effect of numerical instability is comparatively small.

6. Conclusion and Further Research

For Markov chains with a specific transition structure, we have proven that the

Table 3. Numerical values for the M/M/1 queueing system for $\rho = \frac{1}{3}$.

k	Forward computation	GCF based solution	Exact solution
0	1	1	1
1	0.333333	0.3333	0.3333
2	0.111111	0.1111	0.1111
3	0.03704	0.03704	0.03704
4	0.01235	0.01235	0.01235
5	0.004115	0.004115	0.004115
6	0.001372	0.001372	0.001372
7	4.572×10^{-4}	4.572×10^{-4}	4.572×10^{-4}
8	1.524×10^{-4}	1.524×10^{-4}	1.524×10^{-4}
10	1.694×10^{-5}	1.694×10^{-5}	1.694×10^{-5}
12	1.882×10^{-6}	1.882×10^{-6}	1.882×10^{-6}
15	6.969×10^{-8}	6.969×10^{-8}	6.969×10^{-8}
20	2.868×10^{-10}	2.868×10^{-10}	2.868×10^{-10}
25	1.180×10^{-12}	1.180×10^{-12}	1.180×10^{-12}
30	4.870×10^{-15}	4.857×10^{-15}	4.857×10^{-15}
40	1.312×10^{-17}	8.225×10^{-20}	8.225×10^{-20}
50	1.304×10^{-17}	1.393×10^{-24}	1.393×10^{-24}
90	1.304×10^{-17}	1.146×10^{-43}	1.146×10^{-43}

(that is, the corresponding Markov chain is a *quasi-birth-death process*) by means of matrix-valued continued fractions has been studied in [31]. The resulting algorithm is similar to the matrix-analytic methods studied in [32] [33]. An intuitive combination is the study of transition probability matrices of the form (1) where all P_{kl} are matrices. For practical issues, it would be desirable to find a memory-efficient algorithm for computing stationary expectations. For quasi-birth-death processes (that is, block-tridiagonal transition matrices), such a method has been suggested in [34].

- Instead of banded matrices, we could consider upper Hessenberg matrices P (or lower Hessenberg matrices S). Then the difference equation (4) of order n is replaced by a difference equation of infinite order (sometimes referred to as *sum equation*). Furthermore, arbitrary lower bandwidths for P could be considered (as in [9], where the upper bandwidth was restricted to 1).

Acknowledgements

We acknowledge support by Open Access Publishing Fund of Clausthal University of Technology.

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