Application of the One-Step Second-Derivative Method for Solving the Transient Distribution in Markov Chain

Zeina Mueen
Department of Computer Science, College of Science, University of Baghdad, Baghdad, Iraq
zeina.m@uobaghdad.edu.iq (corresponding author)

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ABSTRACT

Markov chains are an application of stochastic models in operation research, helping the analysis and optimization of processes with random events and transitions. The method that will be deployed to obtain the transient solution to a Markov chain problem is an important part of this process. The present paper introduces a novel Ordinary Differential Equation (ODE) approach to solve the Markov chain problem. The probability distribution of a continuous-time Markov chain with an infinitesimal generator at a given time is considered, which is a resulting solution of the Chapman-Kolmogorov differential equation. This study presents a one-step second-derivative method with better accuracy in solving the first-order Initial Value Problems (IVPs) compared to other approaches found in the literature, which is verified by the obtained solutions. The determination of the transient solutions for Markov chains is presented using the proposed method. The results show better accuracy in solving the transient distribution in Markov chains, which implies that there is an improved assurance in adopting this approach in future studies of the Markov chain modeling process for predicting future events based on the current state of a process. Future studies on Markov chain modeling could adopt the introduced method to predict future events based on the current state of a process.

Keywords-transient distribution; Chapman-Kolmogorov; differential equation; numerical method; initial value problem

I. INTRODUCTION

A description of the various states a physical system can occupy represents this system's behavior and specifies its movement in time from one state to another. If the property of exponential distribution applies to the time spent in any state, Markov processes may be used in the representation of the system [1, 2]. In definition, a stochastic process whose conditional probability distribution function satisfies the Markov property is called a Markov process. According to the Markov property, the future evolution of a system depends on its current rather than on its past state [3-5]. The Markov process is referred to as a Markov chain when the state space of the Markov process, which is mostly defined as a set of natural integers or its subset, is discrete [6, 7]. The computation of the probability of being in a given state or subset of states at a certain time after the system becomes operational is usually the main objective when considering Markov chains. The probabilities at a particular time are called transient probabilities and for situations where the number of states is small, one can easily obtain transient solutions which will give information about the behavior of the system, but the solution process becomes more tasking as the models become more complex [1, 8]. The methods being used to obtain transient solutions for Markov chain problems broadly range from the decomposition and matrix-scaling methods [9, 10] to the ODE solvers [11-13] and the uniformization method [11, 14, 15]. According to [12], the use of ODE solvers is more advantageous compared to other methods, because the existing numerical methods for solving ODEs apply to Markov chains whose infinitesimal generators are a function of time, $Q(t)$, that is, to non homogeneous Markov chains. The vector $\pi(t)$ of all such probabilities is given by:

$$\pi(t)=\pi(0)e^{Qt} \tag{1}$$

where e^{Qt} is given by:

$$e^{Qt}=\sum_{k=0}^{\infty}\left(Qt\right)^{k}/k! \tag{2}$$

The vector $\pi(t)$ is the solution of the Chapman-Kolmogorov differential equation:

$$\pi'(t)=\pi(t)Q;\ \pi(t=0)=\pi(0) \tag{3}$$

Equation (3) takes the form of a first-order IVP, which is a type of ODE [16, 17]. Authors in [1] presented some numerical methods that have already been used as ODE solvers in Markov chain problems. These include the Euler method and its variants, which were also studied in [18], where the solutions of transient distribution in Markov chains using trapezoid and Euler methods were explored. In [11], a numerical method was adopted for the solution of a continuous-time Markov chain model implementing the Runge-Kutta and forward Euler methods, while in [19], several methods for obtaining transient solutions were discussed, including the unmodified and modified Euler method. Authors in [1] presented the Taylor series method [20, 21], the Runge-Kutta method [11, 12, 19], and some multistep methods [20, 22, 23].

As observed from the relevant literature, there is a dearth in the studies on ODE solvers to obtain transient solutions in Markov chains. Thus, the current study aims to introduce a new numerical method as an ODE solver for (3). The developed method is a one-step second-derivative method, whose improved accuracy over the existing approaches will be validated by considering certain first-order problems found in the literature and comparing the results to those of existing studies. The flowchart illustrated in Figure 1 shows the phases involved in achieving this paper's objective.

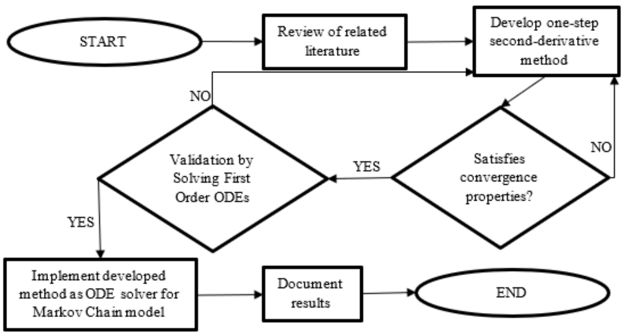

Fig. 1. The solution phases.

II. METHODOLOGY

A. Development of One-Step Second-Derivative Method

To solve the differential equation (3), according to [24], the required linear multistep method will be developed from:

$$\pi_{n+1} = \pi_n + \alpha_0 \pi'_n + \alpha_1 \pi'_{n+1} + \beta_0 \pi''_n + \beta_1 \pi''_{n+1} \tag{4}$$

where α_0, α_1, β_0, and β_1 are the coefficients of the function, π'_n, π'_{n+1}, π''_n, and π''_{n+1} are the first and second derivatives of the function terms, respectively, and the subscript $n+1$ shows the method as a one-step method.

To obtain the values of the coefficients α_0, α_1, β_0, and β_1, the π-terms are individually expanded using Taylor series expansions such that (4) becomes:

$$\begin{aligned}
&\pi(t_n) + h\pi'(t_n) + \frac{h^2}{2}\pi''(t_n) + \frac{h^3}{6}\pi'''(t_n) + \\
&+\frac{h^4}{24}\pi^{(4)}(t_n) + \cdots = \\
&= \pi(t_n) + \alpha_0 \pi'(t_n) + \\
&+\alpha_1\left(\pi'(t_n) + h\pi''(t_n) + \frac{h^2}{2}\pi'''(t_n) + \frac{h^3}{6}\pi^{(4)}(t_n) + \cdots\right) + \\
&+\beta_0 \pi''(t_n) + \beta_1\left(\pi''(t_n) + h\pi'''(t_n) + \frac{h^2}{2}\pi^{(4)}(t_n) + \cdots\right)
\end{aligned} \tag{5}$$

Comparing the coefficients of $\pi^n(t_n)$ and rewriting them in a matrix form gives:

$$\begin{pmatrix} h \\ \frac{h^2}{2} \\ \frac{h^3}{6} \\ \frac{h^4}{24} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & h & 1 & 1 \\ 0 & \frac{h^2}{2} & 0 & h \\ 0 & \frac{h^3}{6} & 0 & \frac{h^2}{2} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \beta_0 \\ \beta_1 \end{pmatrix} \tag{6}$$

The resulting values of α_0, α_1, β_0, and β_1, obtained using the matrix inverse method, are:

$$(\alpha_0, \alpha_1, \beta_0, \beta_1) = \left(\frac{h}{2}, \frac{h}{2}, \frac{h^2}{12}, -\frac{h^2}{12}\right)$$

Therefore, the resulting one-step second-derivative method in (4) is given as:

$$\pi_{n+1} = \pi_n + \frac{h}{2}\pi'_n + \frac{h}{2}\pi'_{n+1} + \frac{h^2}{12}\pi''_n - \frac{h^2}{12}\pi''_{n+1} \tag{7}$$

B. Analysis of Convergence Properties for One-Step Second-Derivative Method

The properties of consistency and zero-stability are the premises to ensure convergence. For the first condition of consistency, a linear multistep method is said to be consistent if it has an order greater than or equal to 1, while the second condition of zero-stability requires that no root of its first characteristic polynomial has a modulus greater than one, and every root with modulus one is simple [24]. To test the consistency of the resultant method in (7), each π-term is expanded using Taylor series expansions such that (7) becomes:

$$\begin{aligned}
&\pi(t_n) + h\pi'(t_n) + \frac{h^2}{2}\pi''(t_n) + \frac{h^3}{6}\pi'''(t_n) + \frac{h^4}{24}\pi^{(4)}(t_n) + \cdots \\
&-\pi(t_n) - \frac{h}{2}\pi'(t_n) - \\
&-\frac{h}{2}\left(\pi'(t_n) + h\pi''(t_n) + \frac{h^2}{2}\pi'''(t_n) + \frac{h^3}{6}\pi^{(4)}(t_n) + \cdots\right) - \\
&-\frac{h^2}{12}\pi''(t_n) + \frac{h^2}{12}\left(\pi''(t_n) + h\pi'''(t_n) + \frac{h^2}{2}\pi^{(4)}(t_n) + \cdots\right) = \\
&= 0
\end{aligned} \tag{8}$$

Then simplifying the coefficients of $\pi^n(t_n)$ on the left-hand-side of the equation gives the following values:

$$\pi(t_n):\pi(t_n)-\pi(t_n)=0$$

$$\pi'(t_n):h-\frac{h}{2}-\frac{h}{2}=0$$

$$\pi''(t_n):\frac{h^2}{2}-\frac{h^2}{2}-\frac{h^2}{12}+\frac{h^2}{12}=0$$

$$\pi'''(t_n):\frac{h^3}{6}-\frac{h^3}{4}+\frac{h^3}{12}=0$$

$$\pi^{(4)}(t_n):\frac{h^4}{24}-\frac{h^4}{12}+\frac{h^4}{24}=0$$

$$\pi^{(5)}(t_n):\frac{h^5}{120}-\frac{h^5}{48}+\frac{h^5}{72}=\frac{h^5}{720}.$$

The first non-zero value was obtained as $h^5/720$, which implies that the one-step second-derivative method is of order 4 with an error constant of 1/720 [24]. Hence, the first condition for the stability of a linear multistep method is satisfied.

On the other hand, the first characteristic polynomial of the method the zero-stability of which is required to be tested is obtained from the non-derivative terms of (7) as $\pi(r) = r - 1$ with roots $r = 1$. Since no root of the first characteristic polynomial has a modulus greater than one, the one-step second-derivative method is zero-stable. Therefore, the method has satisfied all premises required for a linear multistep method to be convergent.

Having justified the convergence of the method, its region of absolute stability is investigated. Considering the one-step second-derivative method in (7), the stability region is obtained by plotting the loci of the roots of the stability polynomial:

$$R(q)=-q+1+z\left(\frac{1}{2}+\frac{q}{2}\right)+z^2\left(\frac{1}{12}-\frac{q}{12}\right) \quad (9)$$

The region of absolute stability is determined by plotting the roots of the polynomial using the boundary locus approach, as depicted in Figure 2.

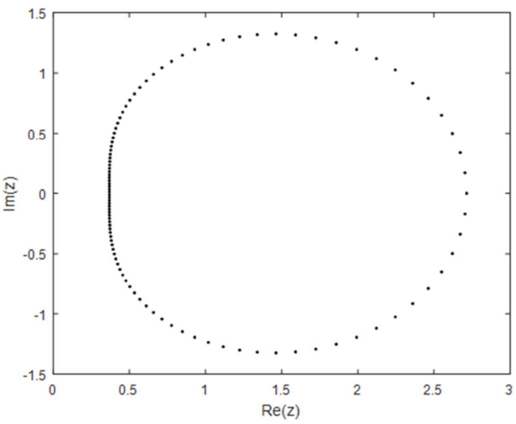

Fig. 2. Region of absolute stability for one-step second-derivative method.

The region outside the line is the stable region of the method. In reference to the definition that a multistep method is A-stable if its region of absolute stability contains the whole of the left-hand half-plane [24, 25], the one-step second-derivative method is A-stable, and therefore suitable for solving first-order IVPs, especially stiff IVPs. Since its basic properties are verified, the accuracy of the developed method is now validated by comparing it with existing methods in the literature for solving first-order IVPs.

C. Solution of First Order IVPs

1) Problem 1 [26]

$$y'(x)=-2100\left(y-\cos(x)\right)-\sin(x),\ y(0)=1,\ x\in[0,1].$$

Exact Solution: $y(x)=\cos x$

Authors in [26] recorded the maximum absolute error obtained at x = 1 with $h = 10^{-1}$, 10^{-2}, and 10^{-3} using a fourth-order method. Comparing the corresponding values with those obtained using a one-step second-derivative method, as shown in Table I, it appears that the latter results in smaller maximum absolute errors of 1.438683e – 11, 5.440093e – 15, and even the same value as the exact solution at $h = 10^{-3}$, with a corresponding maximum absolute error of 0.000000e + 00.

TABLE I. SOLUTION COMPARISON FOR PROBLEM 1

h	Maximum Absolute Error [26]	Maximum Absolute Error (One-Step Second-Derivative Method)
10^{-1}	5.86307e – 7	1.438683e – 11
10^{-2}	5.71593e – 9	5.440093e – 15
10^{-3}	3.33170e – 11	0.000000e + 00

2) Problem 2 [26]

$$y'(x)=-1000000\left(y-\frac{1}{x}\right)-\frac{1}{x^2},\ y(1)=1,\ x\in[1,2].$$

Exact Solution: $y(x)=\frac{1}{x}$

Authors in [26] recorded the maximum absolute error obtained at x = 2 with $h=10^{-1}$, 10^{-2}, and 10^{-3} using an order four/a fourth-order method. Comparing the corresponding values with those obtained using a one-step second-derivative method, as portrayed in Table II, it appears that the second method results in smaller maximum absolute errors of 3.885781e – 15 and 0.000000e + 00, which implies that the same value as that of the exact solution was obtained at $h = 10^{-2}$ and 10^{-3}.

TABLE II. SOLUTION COMPARISON FOR PROBLEM 2

h	Maximum Absolute Error [26]	Maximum Absolute Error (One-Step Second-Derivative Method)
10^{-1}	1.26594e – 8	3.885781e – 15
10^{-2}	1.12913e – 10	0.000000e + 00
10^{-3}	9.95981e – 13	0.000000e + 00

3) Problem 3 [27]

$$y'(x)=1-y^2,\ y(0)=0,\ x\in[0,1].$$

Exact Solution: $y(x)=\dfrac{e^{2x}-1}{e^{2x}+1}$

Authors in [27] recorded the absolute error obtained over the interval with h=0.1 using a three-step order four/fourth-order method. The results obtained using the one-step second-derivative method, were smaller at all points recorded and also displayed better convergence to the exact solution as $x\rightarrow 1$, as outlined in Table III.

4) Problem 4 [28, 29]

$$y'(x)=y,\ y(0)=1,\ x\in[0,1].$$

Exact Solution: $y(x)=e^x$

In both studies [28, 29], authors presented new Runge-Kutta approaches for solving Problem 4, where the former introduced a fifth-stage fourth-order Runge–Kutta formula and the latter developed a four-stage harmonic Runge-Kutta scheme. The one-step second-derivative method outperformed the two Runge-Kutta approaches with smaller absolute error values, as presented in Table IV. This improved accuracy is attributed to the introduction of the higher derivative terms π''_n and π''_{n+1}, in contrast to other approaches that are limited to terms of the form π'_n and π'_{n+1}, when considering first-order IVPs. Hence, based on the obtained results, the validation phase of the one-step second-derivative method for solving first-order ODEs is complete.

TABLE III. SOLUTION COMPARISON FOR PROBLEM 3

x	Exact Solution	Absolute Error [27]	Absolute Error (One-Step Second-Derivative Method)
0.1	0.099667994624955833	2.01e – 06	2.15083e – 07
0.2	0.197375320224904010	1.95e – 06	3.890244e – 07
0.3	0.291312612451590960	1.86e – 06	4.856380e – 07
0.4	0.379948962255224950	3.66e – 06	5.011775e – 07
0.5	0.462117157260009790	3.36e – 06	4.439289e – 07
0.6	0.537049566998035300	3.05e – 06	3.374950e – 07
0.7	0.604367777117163500	2.67e – 06	2.097013e – 07
0.8	0.664036770267848910	2.35e – 06	8.491983e – 08
0.9	0.716297870199024360	2.04e – 06	2.018992e – 08
1.0	0.761594155955764850	1.16e – 06	9.749062e – 08

TABLE IV. SOLUTION COMPARISON FOR PROBLEM 4

x	Absolute Error [28]	Absolute Error [29]	Absolute Error (One-Step Second-Derivative Method)
0.1	3.5914189400e – 8	3.11266882e – 7	1.535873e – 8
0.2	7.9382633800e – 8	9.88006115e – 7	3.394805e – 8
0.3	1.3159706524e – 7	1.14054636e – 6	5.627759e – 8
0.4	1.9391632944e – 7	1.68066466e – 6	8.292848e – 8
0.5	2.6788835550e – 7	2.32177680e – 6	1.145627e – 7
0.6	3.5527489772e – 7	3.07915181e – 6	1.519336e – 7
0.7	4.5807939175e – 7	3.97015331e – 6	1.958980e – 7
0.8	5.7857830127e – 7	5.01451127e – 6	2.474295e – 7
0.9	7.1935638957e – 7	6.23462765e – 6	3.076334e – 7
1.0	8.8334638759e – 7	7.65592021e – 6	3.777638e – 7

III. APPLICATION OF THE ONE-STEP SECOND-DERIVATIVE METHOD TO MARKOV CHAIN

The application of the developed method to the Markov chain is discussed below, using examples from various 3x3 infinitesimal generators. The initial condition and length of the interval of integration are defined, and the results are given in terms of the 2-norm absolute error.

A. Illustrative Example 1 [18]

$$Q=\begin{pmatrix}-2 & 1 & 1\\ 3 & -8 & 5\\ 1 & 2 & -3\end{pmatrix},\ \pi(0)=(1,0,0)\text{ and the length of the}$$

interval of integrations is $t\in[0,1]$ with $h=0.1$

Table V presents the results per iteration for solving the Illustrative Example 1 although the numerical values for some points were not presented in [18]. However, the information required to compute the 2-norm absolute error with respect to the exact solution is available, and hence the 2-norm absolute error is computed. From Table VI, it can be observed that the one-step second-derivative method is more accurate than the approach it was compared with. To further justify the advantage/advantages of the one-step second-derivative method, a second Illustrative Example is considered.

B. Illustrative Example 2 [18]

$$Q=\begin{pmatrix}-3 & 2 & 1\\ 2 & -7 & 5\\ 1 & 1 & -2\end{pmatrix},\ \pi(0)=(1,0,0)\text{ and the length of the}$$

interval of integrations is $t\in[0,1]$ with $h=0.1$

Table VII gives the results per iteration for solving the Illustrative Example 2. The numerical values at all points are presented and the information required to compute the 2-norm absolute error with respect to the exact solution is extracted and utilized for the error computation.

Table VIII shows consistency in the results produced by the one-step second-derivative method. The approach is more accurate than the approach it was compared with, as seen in/by the smaller value of the 2-norm absolute error.

TABLE V. SOLUTION COMPARISON FOR EXAMPLE 1

t	$\pi(t)$ [18]	$\pi(t)$ (One-Step Second-Derivative Method)
0.1	(0.832370,0.072254,0.95376)	(0.8342907645,6.959787892x10^{-2},9.611135661x10^{-2})
0.2	(0.717665,0.105750,0.176585)	(0.7198979374,0.1036960506,0.1764060120)
0.3	(0.637332,0.123417,0.239251)	(0.6394508714,0.1221626589,0.2383864696)
0.4	-	(0.5822915763,0.133144394,0.2845640295)
0.5	-	(0.5414518541,0.1401691768,0.3183789689)
0.6	-	(0.5121851683,0.1448895316,0.3429253000)
0.7	-	(0.4911787108,0.1481581371,0.360663152)
0.8	-	(0.4760884441,0.1504607607,0.3734507951)
0.9	-	(0.4652433341,0.1520983618,0.382658304)
1.0	(0.456848,0.153361,0.389791)	(0.4574473139,0.1532690021,0.3892836839)

TABLE VI. EXACT SOLUTION AND 2-NORM OF ABSOLUTE ERROR FOR EXAMPLE 1

Approach	$\pi(t)$ at t=1	$\|\| \pi(t_1) - \pi_1 \|\|_2$
Exact Solution	(0.457446207856865,0.153269223235319,0.389284568907817)	
[18]	(0.456848,0.153361,0.389791)	7.88907e – 4
One-Step Second-Derivative Method	(0.4574473139,0.1532690021,0.3892836839)	1.433691418e – 6

TABLE VII. SOLUTION COMPARISON FOR EXAMPLE 2

t	$\pi(t)$ [18]	$\pi(t)$ (One-Step Second-Derivative Method)
0.1	(0.7,0.2,0.1)	(0.7592225694,0.1276011605,0.1131762702)
0.2	(0.54,0.21,0.25)	(0.6041647534,0.1719824966,0.22385275)
0.3	(0.445,0.196,0.359)	(0.5022199119,0.1834762187,0.3143038694)
0.4	(0.3866,0.1837,0.4297)	(0.4342171269,0.183036688,0.382746185)
0.5	(0.35033,0.1754,0.47427)	(0.3884073632,0.1790782535,0.4325143832)
0.6	(0.327738,0.170113,0.502149)	(0.3573453443,0.1747557864,0.4678988693)
0.7	(0.3136541,0.1667964,0.5195495)	(0.3361926793,0.1710840927,0.4927232280)
0.8	(0.3048721,0.16472469,0.53040321)	(0.3217478437,0.1682545021,0.5099976542)
0.9	(0.299395729,0.163432148,0.537172123)	(0.3118658673,0.1661765175,0.5219576152)
1.0	(0.295980652,0.162626002,0.541393346)	(0.3050975640,0.1646906318,0.5302118043)

TABLE VIII. EXACT SOLUTION AND 2-NORM OF ABSOLUTE ERROR FOR EXAMPLE 2

Approach	$\pi(t)$ at t=1	$\|\| \pi(t_1) - \pi_1 \|\|_2$
Exact Solution	(0.305095895857673,0.164690716304774,0.530213387837553)	
[18]	(0.295980652,0.162626002,0.541393346)	1.457196556e – 2
One-Step Second-Derivative Method	(0.3050975640,0.1646906318,0.5302118043)	2.301614881e – 6

IV. CONCLUSION

This article has identified the scarcity in the studies on Ordinary Differential Equation (ODE) solvers, with the purpose of developing more accurate approaches for solving the transient distribution in Markov chain problems. For this reason, a one-step second-derivative method was introduced to obtain more accurate solutions than those of previous approaches. The use of higher derivate methods, such as the one-step second-derivative method has been adopted in various studies where it was required to attain approximate solutions to differential equations, especially ODEs. The results of those studies show that the introduction of higher derivatives improves the numerical accuracy of the solutions. Hence, to take advantage of that improved accuracy, a higher derivative method was developed and adopted for the solution of transient distribution in Markov chain models, which is yet to be explored in the literature. To justify the usability of the developed method, the latter was verified for convergence and validated by having been compared with existing methods for solving first-order Initial Value Problems (IVPs). The considered first-order IVPs included both linear and nonlinear IVPs. From the results it is observed that as ????? tends to zero, the accuracy of the one-step second-derivative method increased such that the solution obtained became the same as the exact solution. This affirms that the zero-stability property was satisfied by the proposed method. Furthermore, a better accuracy over the existing methods was also observed. Based on its performance in solving first-order IVPs, the one-step second-derivative method was then implemented as an ODE solver for the selected Markov chain problems. The 2-norm absolute error for both Illustrative Examples considered was displayed. The one-step second-derivative method obtained better and smaller errors in both examples. Overall, the proposed one-step second-derivative method's has demonstrated better accuracy for solving first-order IVPs in general and it is also suitable for application to obtain an approximate solution for transient distribution in the Markov chain. Its practical application to Markov chains and its extension to non-Markovian or more complex stochastic models can be considered in future studies.

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