



The Application of Runge-Kutta and Backward Differentiation Methods for Solving Transient Distribution in Markov Chain

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ABSTRACT

The computation of state probability distributions at an arbitrary point in time, which in the case of a discrete-time Markov chain means finding the distribution at some arbitrary time step n denoted $\pi^{(n)}$, a row vector whose i^{th} component is the probability that the Markov chain is in state i at time step n , is the iterative solution methods for transient distribution in Markov chain. The solutions of transient distribution in Markov chain using Euler and trapezoid methods have been investigated in this study, in order to provide some insight into the solutions of transient distribution in Markov chain, which produce a significantly more accurate response in less time for some types of situations and also tries to get to the end result as quickly as possible while the solution must be computed when a specified number of well-defined stages have been completed.

1. INTRODUCTION

The solution of ordinary differential equations (ODEs) has triggered a lot of interest (and continues to do so), and there are a lot of ways to use ODE procedures to compute transient solutions of Markov chains. Numerical methods for the

Received: 01/09/2021, Accepted: 21/10/2021, Revised: 25/11/2021. * Corresponding author.
2015 *Mathematics Subject Classification*. 46H99 & 43A10.

Keywords and phrases. Chapman-Kolmogorov equation, eigenvalues, Jacobian, Gerschgorin disk theorem, infinitesimal generator, Runge-Kutta, backward differentiation formulae

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solution of ODEs, unlike uniformization and matrix scaling and powering, are applicable to nonhomogeneous Markov chains, i.e., Markov chains whose infinitesimal generators are a function of time, $Q(t)$. However, because the field of ordinary differential equations is so large, our goal in this study is to provide only the most basic introduction to this method. In the discipline of numerical analysis, there are two types of solution methods: iterative solution methods and direct solution methods. Iterative approaches start with an initial estimate of the solution vector and then alter it in such a way that it gets closer and closer to the genuine solution with each step or iteration. It eventually converges on the true solution. If there is no known initial approximation, a guess is performed or an arbitrary initial vector is used instead. The solution must be computed when a specified number of well-defined stages have been completed. For large-scale Markov chains, methods currently used to obtain transient solutions are based either on readily available differential equation solvers such as the Adams formulae and backward differentiation formulae (BDF). Most of these methods experience difficulty when both $\max_j |q_{jj}|$ (the largest exit rate from any state) and t (the time at which the solution is required) are large, and there appears to be little to recommend a single method for all situations. In this study we discuss the Runge-Kutta and Backward Differentiation Formulae methods. These methods are extremely simple to program and often outperforms other methods, and the two methods are useful particularly if the solution is required at many points, or if plots need to be drawn to show the evolution of certain performance measures. [15] established the application and simulation of discrete Markov Chains and [10] explain the nineteen dubious ways to compute the exponential of a matrix while [16] explained the degree of the best rational approximation to the exponential function and [21] explained the numerical Computation of the Matrix Exponential with Accuracy Estimate. [13] & [14] illustrated a stable recursion for the Steady State Vector in Markov chains of M/G/1 type while [12] derived the transient solution of Markov Processes by Krylov Subspaces, [9] described the permuting Markov chains to nearly completely decomposable form. whereas [17] & [18] discussed the development of Numerical Solutions of Markov chains, while [11] demonstrated the appropriateness of the Markov chain technique in the wind feed in Germany (2015) and [1] demonstrated the batch processes in machine repair problem while [19] used the Markov chain model of fuzzy state to anticipate the direction of gold price movement and to estimate the probabilistic transition matrix of gold price closing returns, whereas [7] used the Markov chain model of fuzzy state to predict monthly rainfall data while [8] demonstrated the application of Markov chain to the spread of disease infection, demonstrating that Hepatitis B became more infectious over time than tuberculosis and HIV and [20] demonstrated the application of Markov chain to journalism. [2] introduced

direct equation solving algorithms compositions of lower -upper triangular matrix and Grassmann–Taksar–Heyman for the stationary distribution of Markov chains while [5] analysed the matrix geometric and analytical block numerical iterative methods for stationary distribution in the structured Markov chains. [4] demonstrated the performance measure analysis on the states classification in Markov chain while [6] established the application of renewal reward processes in homogeneous discrete Markov chain and, [3] discussed the decomposition and aggregation algorithmic numerical iterative solution methods for the stationary distribution of Markov chain. However, However, in this study, the application of Runge-Kutta and backward differentiation formulae (BDF) methods of solving transient distribution in Markov chain is considered with illustrative examples.

- 1.1. **Notation.** $\pi_{(i+1)}$, Runge-Kutta and backward differentiation formulae solution method;
 h_i , step size at step i ; $\pi(t)$, is the transient solution at time t ;
 π , is the stationary distribution; Q , infinitesimal generator; z_{i+1} , finite element method;
 $z^I = g(t)$, first-order differential equation and
 $z(t)$, is the row vector $\pi(t)$ of the solution in Markov chain with function $g(t, z(t))$;
 p , order of derivative;
 θ and γ , chosen constants; λ_k , eigen value

2. METHODOLOGY

The Runge-Kutta methods are a very important and effective class of single step procedures. The accuracy of a Runge-Kutta algorithm of order p is comparable to that of a Taylor series algorithm of order p , but without the requirement to find and evaluate the derivatives $g', g'', g''', \dots, g^{(p-1)}$, instead requiring the assessment of $g(t, z)$ at selected points. A comparison with the terms through h^p in the Taylor series technique for the first step, i.e. the computation of z_1 from the initial condition (t_0, z_0) , yields an order p Runge–Kutta method.

Because the analysis presupposes that the value around which the expansion is conducted is known precisely, this is the case. If the Taylor series for the exact solution $z(t_0 + h)$ and the Taylor series for the calculated solution z^I coincide up to and including the term h^p , the Runge–Kutta technique is said to be of order p . A Runge–Kutta technique of order 2 (RK2), for example, is meant to provide the same order of convergence as a Taylor series approach of order 2 without requiring differentiation. It's written like this:

$$(1) \quad z_{i+1} = z_i + h (ak_1 + bk_2),$$

where a and b are constants

$$k_1 = g(t_i, z_i),$$

$$(2) \quad k_2 = g(t_i + \theta h, z_i + \gamma h k_1).$$

and θ and γ are constants.

Through the term in h^2 , the constants are chosen so that the Taylor series approach corresponds with (1) at $i = 0$. Calculating the derivatives of (1) at $i = 0$ and comparing coefficients with those of the first and second derivatives derived from the accurate Taylor series expansion are required to get these constants. The constants a , b , θ , γ :

$$a + b = 1, \quad \theta b = \gamma b = \frac{1}{2}.$$

These are satisfied by the choice $a = b = \frac{1}{2}$ and $\theta = \gamma = 1$, so the resulting RK2 method is

$$z_{i+1} = z_i + \frac{h}{2}g(t_i, z_i) + \frac{h}{2}g(t_i + h, z_i + hg(t_i, z_i)).$$

There are other more options for the constants. Order 4 Runge-Kutta procedures are the most widely used. The standard RK4 technique, which is given by, requires four function evaluations per step.

$$(3) \quad z_{i+1} = z_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$

$$k_1 = g(t_i, z_i),$$

$$k_2 = g\left(t_i + \frac{h}{2}, z_i + \frac{h}{2}k_1\right),$$

$$k_3 = g\left(t_i + \frac{h}{2}, z_i + \frac{h}{2}k_2\right),$$

$$(4) \quad k_4 = g(t_i + h, z_i + hk_3).$$

It is worth noting that each k_i represents a point in the (t, z) plane where g must be evaluated. Each one is known as a stage. As a result, (3) describes a fourth-order, four-stage, explicit Runge-Kutta approach. When the Chapman–Kolmogorov equations $\pi^I = \pi Q$ are solved using the typical explicit fourth-order Runge–Kutta technique given by (3), the sequence of operations to be conducted to go from $\pi_{(i)}$ to the next time step $\pi_{(i+1)}$ is as follows:

$$(5) \quad \pi_{(i+1)} = \pi_{(i)} + h(k_1 + 2k_2 + 2k_3 + k_4)/6,$$

$$k_1 = \pi_{(i)}Q$$

$$k_2 = \left(\pi_{(i)} + \frac{h}{2}k_1\right)Q,$$

$$k_3 = \left(\pi_{(i)} + \frac{h}{2}k_2\right)Q,$$

$$k_4 = (\pi_{(i)} + hk_3)Q.$$

3. RESULTS AND DISCUSSION

This section discusses the solutions to the performance measures such as transient distribution, error terms and interpolating polynomial constant terms *etc.* of Runge-Kutta and backward differentiation formulae (BDF) methods using illustrative examples

Illustrative Example 1: Consider a continuous-time Markov chain with infinitesimal generator

$$Q = \begin{pmatrix} -3 & 2 & 1 \\ 2 & -7 & 5 \\ 1 & 1 & -2 \end{pmatrix}.$$

Assume we want to extract the transient distribution using the Runge-Kutta of fourth-order, four-stage (RK4) approach. At time $t = 1$, the Markov chain starts in state 1 with $\pi_{(0)} = (1 \ 0 \ 0)$ With a fixed step size of 0.1, calculate $\pi_{(i)}$, $i = 1, 2, \dots, 10$.

$$k_1 = \pi_{(0)}Q = (1 \ 0 \ 0) \begin{pmatrix} -3 & 2 & 1 \\ 2 & -7 & 5 \\ 1 & 1 & -2 \end{pmatrix} = (-3 \ 2 \ 1),$$

$$\begin{aligned} k_2 = (\pi_{(0)} + 0.05k_1)Q &= (0.85 \ 0.1 \ 0.05) \begin{pmatrix} -3 & 2 & 1 \\ 2 & -7 & 5 \\ 1 & 1 & -2 \end{pmatrix} \\ &= (-2.3 \ 1.05 \ 1.25), \end{aligned}$$

$$\begin{aligned} k_3 = (\pi_{(0)} + 0.05k_2)Q &= (0.885 \ 0.0525 \ 0.0625) \begin{pmatrix} -3 & 2 & 1 \\ 2 & -7 & 5 \\ 1 & 1 & -2 \end{pmatrix} \\ &= (-2.4875 \ 1.465 \ 1.0225), \end{aligned}$$

$$\begin{aligned} k_4 = (\pi_{(0)} + 0.1k_3)Q &= (0.75125 \ 0.1465 \ 0.10225) \begin{pmatrix} -3 & 2 & 1 \\ 2 & -7 & 5 \\ 1 & 1 & -2 \end{pmatrix} \\ &= (-1.8585 \ 0.57925 \ 1.27925). \end{aligned}$$

which allows us to compute

$$\pi(0.1) \approx \pi_{(1)} = \pi_{(0)} + \frac{h(k_1 + 2k_2 + 2k_3 + k_4)}{6}$$

where

$$\begin{aligned} \frac{h(k_1 + 2k_2 + 2k_3 + k_4)}{6} &= \frac{0.1 \begin{pmatrix} -14.433 & 7.60925 & 6.82425 \end{pmatrix}}{6} \\ &= 0.1 \begin{pmatrix} -2.4055 & 1.268208333 & 1.137375 \end{pmatrix} \end{aligned}$$

$$= (-0.24055 \quad 0.126821 \quad 0.1137375)$$

Therefore,

$$\begin{aligned} \pi(0.1) &\approx \pi_{(1)} = (1 \quad 0 \quad 0) + (-0.24055 \quad 0.126821 \quad 0.1137375) \\ &= (0.75945 \quad 0.126821 \quad 0.1137375), \end{aligned}$$

$$\begin{aligned} \pi(0.2) &\approx \pi_{(2)} = (0.75945 \quad 0.126821 \quad 0.1137375) + (-0.24055 \quad 0.126821 \quad 0.1137375) \\ &= (0.5089 \quad 0.253642 \quad 0.227475), \end{aligned}$$

$$\begin{aligned} \pi(0.3) &\approx \pi_{(3)} = (0.5089 \quad 0.253642 \quad 0.227475) + (-0.24055 \quad 0.126821 \quad 0.1137375) \\ &= (0.26835 \quad 0.380463 \quad 0.3412125), \end{aligned}$$

$$\begin{aligned} \pi(0.4) &\approx \pi_{(4)} = (0.26835 \quad 0.380463 \quad 0.3412125) + (-0.24055 \quad 0.126821 \quad 0.1137375) \\ &= (0.0278 \quad 0.507284 \quad 0.45495), \end{aligned}$$

$$\begin{aligned} \pi(0.5) &\approx \pi_{(5)} = (0.0278 \quad 0.507284 \quad 0.45495) + (-0.24055 \quad 0.126821 \quad 0.1137375) \\ &= (-0.21275 \quad 0.634105 \quad 0.568688), \end{aligned}$$

Since $\pi(0.5) \approx \pi_{(5)}$ contain the negative result, hence, $\pi(0.4) \approx \pi_{(4)}$
 $= (0.0278 \quad 0.507284 \quad 0.45495)$ is the transient solution.

Illustrative Example 2: Consider the continuous-time Markov chain given below. apply the Runge-Kutta of fourth-order, four-stage (RK4) method to obtain the transient distribution. With $\pi_{(0)} = (1 \quad 0 \quad 0)$ and

$$Q = \begin{pmatrix} -2 & 1 & 1 \\ 3 & -8 & 5 \\ 1 & 2 & -3 \end{pmatrix},$$

we find, taking steps of size .1,

$$k_1 = \pi_{(0)}Q = (1 \quad 0 \quad 0) \begin{pmatrix} -2 & 1 & 1 \\ 3 & -8 & 5 \\ 1 & 2 & -3 \end{pmatrix} = (-2 \quad 1 \quad 1),$$

$$k_2 = (\pi_{(0)} + 0.05k_1)Q = (0.9 \quad 0.5 \quad 0.5) \begin{pmatrix} -2 & 1 & 1 \\ 3 & -8 & 5 \\ 1 & 2 & -3 \end{pmatrix} = (-1.6 \quad 0.6 \quad 1),$$

$$k_3 = (\pi_{(0)} + 0.05k_2)Q = (0.92 \quad 0.03 \quad 0.05) \begin{pmatrix} -2 & 1 & 1 \\ 3 & -8 & 5 \\ 1 & 2 & -3 \end{pmatrix} = (-1.7 \quad 0.78 \quad 0.92),$$

$$k_4 = (\pi_{(0)} + 0.1k_3)Q = (0.83 \quad 0.078 \quad 0.092) \begin{pmatrix} -2 & 1 & 1 \\ 3 & -8 & 5 \\ 1 & 2 & -3 \end{pmatrix} = (-1.334 \quad 0.39 \quad 0.944).$$

which allows us to compute (2),

where $\frac{h(k_1+2k_2+2k_3+k_4)}{6} = \frac{0.1 \begin{pmatrix} -9.934 & 4.15 & 5.784 \end{pmatrix}}{6} = \begin{pmatrix} -0.165567 & 0.069167 & 0.0964 \end{pmatrix}$.

Therefore,

$$\begin{aligned} \pi(0.1) &\approx \pi_{(1)} = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} + \begin{pmatrix} -0.165567 & 0.069167 & 0.0964 \end{pmatrix} \\ &= \begin{pmatrix} 0.834433 & 0.069167 & 0.0964 \end{pmatrix}, \\ \pi(0.2) &\approx \pi_{(2)} = \begin{pmatrix} 0.834433 & 0.069167 & 0.0964 \end{pmatrix} + \begin{pmatrix} -0.165567 & 0.069167 & 0.0964 \end{pmatrix} \\ &= \begin{pmatrix} 0.668866 & 0.138334 & 0.1928 \end{pmatrix}, \\ \pi(0.3) &\approx \pi_{(3)} = \begin{pmatrix} 0.668866 & 0.138334 & 0.1928 \end{pmatrix} + \begin{pmatrix} -0.165567 & 0.069167 & 0.0964 \end{pmatrix} \\ &= \begin{pmatrix} 0.503299 & 0.207501 & 0.2892 \end{pmatrix}, \\ \pi(0.4) &\approx \pi_{(4)} = \begin{pmatrix} 0.503299 & 0.207501 & 0.2892 \end{pmatrix} + \begin{pmatrix} -0.165567 & 0.069167 & 0.0964 \end{pmatrix} \\ &= \begin{pmatrix} 0.337732 & 0.276668 & 0.3856 \end{pmatrix}, \\ &\vdots \\ \pi(1.0) &\approx \pi_{(10)} = \begin{pmatrix} 0.097182 & 0.403489 & 0.4993375 \end{pmatrix}, \end{aligned}$$

and the final error is

$$\|\pi(1.0) - \pi_{(10)}\|_2 = 0.00001256.$$

Stiffness is an important property of initial-value ordinary differential equations ODEs. Stiff ODEs are extremely difficult to solve using explicit methods, to the point where one definition of stiff equations is "problems for which explicit methods fail." The eigenvalues of the Jacobian $\frac{\partial g}{\partial z}$ and the length of the integration interval are two elements that influence stiffness. The difficulties arise from the presence of rapidly decaying transient terms in the solutions of stiff systems of differential equations.

Illustrative Example 3: Consider the infinitesimal generator

$$Q = \begin{pmatrix} -1 & 1 \\ 100 & -100 \end{pmatrix}$$

with initial probability vector $\pi_{(0)} = \begin{pmatrix} 1 & 0 \end{pmatrix}$, Q has the decomposition

$Q = S\lambda S^{-1}$ where

$$S = \begin{pmatrix} 1 & -0.01 \\ 1 & 1 \end{pmatrix} \text{ and } \lambda = \begin{pmatrix} 0 & 0 \\ 0 & -101 \end{pmatrix}.$$

Since

$$\pi_{(t)} = \pi_{(0)}e^{Qt} = \pi_{(0)}Se^{\lambda t}S^{-1},$$

we find that

$$\pi_{(t)} = \frac{1}{1.01} (e^0 + 0.01e^{-101t}, 0.01e^0 - 0.01e^{-101t}),$$

In this expression, the exponents e^{-101t} tend to zero quickly, leaving the stationary probability distribution. Despite this, when using an explicit technique,

small step sizes must be employed throughout the integration phase. Once the terms in e^{-101t} are virtually zero, it is impossible to raise the step size. When particular eigenvalues of the Jacobian matrix (with elements $\frac{\partial g_i}{\partial z_i}$) have substantial negative real parts when compared to others, a system of ODEs is said to be stiff, according to the classical definition.

When $\underbrace{Max}_k |Re(\lambda_k)| \gg 0$, Markov chain issues (where the Jacobian is given by Q , the infinitesimal generator) are stiff, according to this definition. This amount can be bound using the Gerschgorin disk theorem. This conclusion follows from the specific features of infinitesimal generator matrices.

$$(6) \quad \underbrace{Max}_k |Re(\lambda_k)| \leq 2 \underbrace{Max}_j |q_{jj}|,$$

i.e., twice the largest total exit rate from any one state in the Markov chain.

Illustrative Example 4: Consider a Markov chain with infinitesimal generator

$$Q = \begin{pmatrix} -2 & 1 & 1 \\ 3 & -8 & 5 \\ 1 & 2 & -3 \end{pmatrix}$$

The implicit ($k = 2$) backward differentiation formulae (BDF formula) will be used. When using the trapezoid rule, we need to keep in mind that. We shall apply the implicit ($k = 2$) backward differentiation formulae (BDF formula).

When applying the trapezoid rule

$$\begin{aligned} \pi_{(i+1)} &= \pi_i \left(I + \frac{h_{i+1}}{2} Q \right) \left(I - \frac{h_{i+1}}{2} Q \right)^{-1} = \pi_i \begin{pmatrix} 0.9 & 0.05 & 0.05 \\ 0.15 & 0.60 & 0.25 \\ 0.05 & 0.10 & 0.85 \end{pmatrix} \\ &\quad \begin{pmatrix} 1.10 & -0.05 & -0.05 \\ -0.05 & 1.40 & -0.25 \\ -0.05 & -0.1 & 1.15 \end{pmatrix}^{-1} \\ \pi_{(i+1)} &= \pi_i \begin{pmatrix} 0.832370 & 0.072254 & 0.95376 \\ 0.213873 & 0.459538 & 0.326590 \\ 0.096266 & 0.130058 & 0.771676 \end{pmatrix}. \end{aligned}$$

Beginning with $\pi_{(0)} = (1 \ 0 \ 0)$, this allows us to compute

$$\pi(0.1) \approx \pi_{(1)} = (0.832370 \ 0.072254 \ 0.95376),$$

We now have the two starting points for the implicit backward differentiation formulae: $\pi_{(0)} = (1 \ 0 \ 0)$ and $\pi_{(1)} = (0.832370 \ 0.072254 \ 0.95376)$.

We begin with computing.

$$S = (1.5I - 0.1Q)^{-1} = \left[\begin{pmatrix} 1.5 & 0 & 0 \\ 0 & 1.5 & 0 \\ 0 & 0 & 1.5 \end{pmatrix} - 0.1 \begin{pmatrix} -2 & 1 & 1 \\ 3 & -8 & 5 \\ 1 & 2 & -3 \end{pmatrix} \right]^{-1},$$

$$S = \left[\begin{pmatrix} 1.5 & 0 & 0 \\ 0 & 1.5 & 0 \\ 0 & 0 & 1.5 \end{pmatrix} - \begin{pmatrix} -0.2 & 0.1 & 0.1 \\ 0.3 & -0.8 & 0.5 \\ 0.1 & 0.2 & -0.3 \end{pmatrix} \right]^{-1} = \begin{pmatrix} 1.7 & -0.1 & -0.1 \\ -0.3 & 2.3 & -0.5 \\ -0.1 & -0.2 & 1.8 \end{pmatrix}^{-1}$$

$$S = \begin{pmatrix} 0.595870 & 0.029485 & 0.041298 \\ 0.087021 & 0.449853 & 0.129794 \\ 0.042773 & 0.051622 & 0.572271 \end{pmatrix}.$$

We now proceed using (??) for computing

$$\begin{aligned} \pi(0.2) \approx \pi_{(2)} &= (2\pi_{(1)} - 0.5\pi_{(0)}) S = (0.714768 \quad 0.109213 \quad 0.176019), \\ \pi(0.3) \approx \pi_{(3)} &= (2\pi_{(2)} - 0.5\pi_{(1)}) S = (0.623707 \quad 0.127611 \quad 0.239682), \\ &\vdots \\ \pi(1.0) \approx \pi_{(10)} &= (2\pi_{(9)} - 0.5\pi_{(8)}) S = (0.454655 \quad 0.153688 \quad 0.391657). \end{aligned}$$

and the final error is

$$\|\pi(1.0) - \pi_{(10)}\|_2 = 0.003687$$

Conclusion: Solutions for large state spaces using Runge-Kutta and backward differentiation formulae (BDF) methods were computed, which begin with an initial estimate of the solution vector and then alter it in such a way that it gets closer and closer to the true solution with each step or iteration, saving time. Matrices operations, such as the product and matrix inversion are performed and Markov chain laws, theorems, formulas are utilized. For illustrative examples, the transient distribution vector's $\pi_{(i+1)}$, $i = 0, 1, 2, \dots$; is computed for Runge-Kutta and Backward Differentiation Formulae (BDF) with their corresponding error when compared with different method. The importance of multistep backward differentiation formulae (BDF) method in solving stiff systems (ordinary differential equations) was demonstrated, and it was asserts that a system of ODEs is stiff when certain eigenvalues of the Jacobian matrix (with elements $\frac{\partial g_i}{\partial z_i}$) have large negative real parts when compared to others. Also, it was concluded that the solutions of stiff systems of differential equations contain rapidly decaying transient terms.

Acknowledgement: The authors are very grateful to Nigeria Army University Biu and University of Lagos for the supports they received during the compilation of this work and to anonymous referees for their careful reading of the paper and helpful suggestions.

Competing interests: The authors declare that they have no competing interests.

Funding: We declare that no funding from external bodies was received for this research.

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