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IMPROVING RATE OF CONVERGENCE OF AN ITERATIVE SCHEME WITH EXTRA SUB-STEPS FOR TWO STAGE GAUSS METHOD

R. Vigneswaran[1] §, S. Kajanthan[2]

[1]Department of Mathematics and Statistics
Faculty of Science
University of Jaffna
SRI LANKA

[2]Department of Mathematics and Computer Science
Faculty of Natural Sciences
Open University of Sri Lanka

Abstract: The non-linear equations, when implementing implicit Runge-Kutta methods, may be solved by a modified Newton scheme and by several linear iteration schemes which sacrificed superlinear convergence for reduced linear algebra costs. A linear scheme of this type was proposed, which requires some additional computation in each iteration step. The rate of convergence of this scheme is examined when it is applied to the scalar test problem $x' = qx$ and the convergence rate depends on the spectral radius $\rho[M(z)]$ of the iteration matrix M, a function of $z = hq$, where h is a step size. The supremum of the lower bound for $\rho[M(z)]$ is minimized over left-half plane of the z-complex plane and over the negative real axis of the z-plane in order to improve the rate of convergence of that scheme. Two new schemes are obtained for the two stage Gauss method and numerical results are given.

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§Correspondence author

1. Introduction

There are two general approaches proposed by several authors to the implementation of implicit s-stage Runge-Kutta methods to integrate a stiff system of n ordinary differential equations. In one approach, a modified Newton scheme is used and each step of this scheme requires the solution of a set of sn linear equations which is expensive. In this approach, schemes are developed to solve these linear equations efficiently, [6], [1], [7]. In another scheme of this general type, due to Butcher [2], a similarity transformation of the coefficient matrix of the method is used. That is particularly effective when the coefficient matrix has a single point spectrum. To deal with methods where the coefficient matrix has a more general spectrum, Enright [12] proposed the use of an additional similarity transformation to transform the Jacobian matrix of the differential system to Hessenberg form. This scheme is comparatively inefficient when $n > s$ since each of the corresponding vector transformations requires $O(s^2n + sn^2)$ operations. Varah [21] proposed the use of complex arithmatics to deal with the case where the coefficient matrix of the method has a complex spectrum. In final proposal of this first general type, Cash [5] proposed a family of implicit Runge-Kutta methods of a special form which again makes the system of equations effectively of lower dimension. Butcher and Cash [4] developed a special class of implicit Runge-Kutta methods for stiff initial value problems and these methods were derived from known singly implicit methods by adding one or more extra diagonally implicit stages.

The other approach is to use schemes based directly on iterative procedures. Frank and Ueberhuber [13] describe the use of iterated defect correction and a variety of schemes have been discussed by Butcher [3]. He suggested how higher order methods could be used in combination with diagonally implicit methods through an iterated defect correction process. Cooper and Butcher [8] considered a more general scheme which explicitly uses the Jacobian of differential system. Cooper and Vignesvaran [9] developed an alternative scheme which is computationally more efficient. Improved rates of convergence of this scheme were obtained in [22], [23], [24]. Another scheme was proposed by Cooper and Vignesvaran [10] in order to obtain improved rate of convergence, by adding extra sub-steps. Gonzalez, Gonzalez and Montijano [17] proposed a scheme for Gauss methods using an iterative procedure of semi-implicit type in which the Jacobian does not appear explicitly. A scheme of this type was proposed in [18] in which convergence and stability properties of the scheme are discussed in detail. In this paper, the scheme proposed in [10] is discussed further and improved rates of convergence are obtained. Results are obtained only for the

two-stage Gauss method and, in Section 4, some numerical results are given.

2. Motivation

We consider an initial value problem for stiff system of $n(\geq 1)$ ordinary differential equations

$$x' = f(x(t)), \quad x(t_0) = x_0, \quad f : \mathbb{R}^n \to \mathbb{R}^n, \tag{1}$$

where f is assumed to be as smooth as necessary. An s-stage implicit Runge-Kutta method computes an approximation x_{r+1} to the solution $x(t_{r+1})$ at grid point $t_{r+1} = t_r + h$ by

$$x_{r+1} = x_r + h \sum_{i=1}^{s} b_i f(y_i)$$

where the internal approximations $y_1, y_2, \cdots, y_s$ satisfy the sn equations

$$y_i = x_r + h \sum_{j=1}^{s} a_{ij} f(y_j), \quad i = 1, 2, \cdots, s, \tag{2}$$

$A = [a_{ij}]$ is the real coefficient matrix and $b = (b_1, b_2, \cdots, b_s)^T$ is the column vector of the Runge-Kutta method. Let $Y = y_1 \oplus y_2 \oplus \cdots \oplus y_s \in \mathbb{R}^{sn}$ and let $F(Y) = f(y_1) \oplus f(y_2) \oplus \cdots \oplus f(y_s) \in \mathbb{R}^{sn}$. Then equation (2) may be represented by the compact form

$$Y = e \otimes x_r + h(A \otimes I_n)F(Y) \tag{3}$$

where $e = (1, 1, \cdots, 1)^T$ and $A \otimes I_n$ is the Kronecker product of the matrix A with $n \times n$ identity matrix I_n and, in general $A \otimes B = [a_{ij}B]$. This paper deals with methods suitable for stiff systems so that the matrix A is not strictly lower triangular and, in particular, is concerned with Gauss methods of maximum order.

Equation (3) may be solved by a modified Newton iteration. Let J be the Jacobian of f evaluated at some recent point x_r, updated infrequently. The modified Newton scheme evaluates $Y^1, Y^2, Y^3, \cdots$, to satisfy

$$(I_{sn} - hA \otimes J)(Y^m - Y^{m-1}) = D(Y^{m-1}), \quad m = 1, 2, \cdots, \tag{4}$$

where D is the approximation defect, $D(Z) = e \otimes x_r - Z + h(A \otimes I_n)F(Z)$. In each step of this iteration, a set of sn linear equations has to be solved.

For a singly implicit method, there is a non-singular matrix S so that $S^{-1}AS = \lambda(I_s - L)^{-1}$, where L is zero except for some ones on the sub-diagonal. On applying this transformation, the scheme (4) becomes

$$\begin{aligned} [I_s \otimes (I_n - h\lambda J)]E^m &= [(I_s - L)S^{-1} \otimes I_n]D(Y^{m-1}) + (L \otimes I_n)E^m, \\ Y^m &= Y^{m-1} + (S \otimes I_n)E^m, \quad m = 1, 2, 3 \cdots \cdot \end{aligned} \tag{5}$$

Cooper and Butcher [8] proposed an iterative scheme, sacrificing superlinear convergence for reduced linear algebra cost, which may be regarded as a generalization of the scheme (5) for singly implicit methods. They considered the scheme

$$\begin{aligned} [I_s \otimes (I_n - h\lambda J)]E^m &= (B_1 S^{-1} \otimes I_n)D(Y^{m-1}) + (L_1 \otimes I_n)E^m, \\ Y^m &= Y^{m-1} + (S \otimes I_n)E^m, \quad m = 1, 2, \cdots, \end{aligned} \tag{6}$$

where B_1 and S are real $s \times s$ non-singular matrices and L_1 is strictly lower triangular matrix of order s, and λ is a real constant. Peat and Thomas [20], after extensive numerical experiments, concluded that the schemes proposed by Cooper and Butcher are, in general, the most efficient schemes for integration of stiff problems. Gladwell and Thomas [16] recommended this scheme for the two-stage Gauss method. Cooper and Vignesvaran [10] proposed a scheme which is a generalization of the basic scheme (6). They considered the scheme

$$\begin{aligned} [I_r \otimes (I_n - h\lambda J)]E^m &= (BS^{-1} \otimes I_n)D(Y^{m-1}) + (L \otimes I_n)E^m, \\ Y^m &= Y^{m-1} + (SR \otimes I_n)E^m, \quad m = 1, 2, 3, \cdots, \end{aligned} \tag{7}$$

where B and R^T are real $r \times s$ matrices ($r > s$), each of column rank s, and L is a strictly lower triangular matrix of order r. In this scheme, $E^m = E_1^m \oplus E_2^m \oplus \cdots \oplus E_r^m$ is computed and then $Y^m = y_1^m \oplus y_2^m \oplus \cdots \oplus y_s^m$ is computed in each step of the iteration. It has been shown in [10] that if (E^m) has limit zero, then (Y^m) has a limit Y such that $D(Y) = 0$. In this scheme, each step of the iteration still requires s function evaluations but consists of r sub-steps so that there are additional linear algebra cost for solving additional $r - s$ sets of linear equations in each step.

The convergence rate of the scheme is examined when it is applied to the scalar problem $x' = qx$, with rapid convergence required for all $z \in \mathbb{C}^-$, where $\mathbb{C}^- = \{z \mid \Re(z) \leq 0\}$. Let $\Delta^m = (S^{-1} \otimes I_n)(Y - Y^m)$. Then the scheme (7) applied to this test problem gives

$$\Delta^m = M(z)\Delta^{m-1}, \quad m = 1, 2, 3, \cdots,$$

where Y is the solution of $D(Y) = 0$ and M is the iteration matrix given by

$$M(z) = I_s - R[(1-\lambda z)I_r - L]^{-1}B(I_s - z\overline{A}), \quad \overline{A} = S^{-1}AS. \tag{8}$$

Cooper and Vignesvaran [10] considered the partitioned form of the parameter matrices as follows:

$$B = \begin{bmatrix} I_s \\ B_{21} \end{bmatrix} B_{11}, \quad L = \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix}, \quad R = [I_s, R_{12}], \tag{9}$$

where B_{11} is an $s \times s$ non-singular matrix with $\beta = \det B_{11}$ and, L_{11} and L_{22} are strictly lower triangular matrix of order s and $r-s$ respectively. With this partitioning, M may be written as

$$M(z) = I_s - P(z)Q(z), \tag{10}$$

where

$$\begin{aligned} P(z) &= I_s + R_{12}[(1-\lambda z)I_{r-s} - L_{22}]^{-1}[L_{21} + B_{21}(1-\lambda z)I_s - L_{11}], \\ Q(z) &= [(1-\lambda z)I_s - L_{11}]^{-1}B_{11}(I_s - z\overline{A}). \end{aligned} \tag{11}$$

Cooper and Vignesvaran [10] considered the case $r = s+1$ only. For this case, $L_{22} = 0$ and $B_{21} = u^T$ is a row vector and $R_{12} = \eta$ is a column vector. Define $v^T = L_{21} - B_{21}L_{11}$.

Cooper and Vignesvaran [10] considered the two-stage Gauss method and imposed the condition that M has one non zero eigenvalue, so that the spectral radius depends only on three parameters. These parameters were obtained by considering the problem

$$\min \sup_{z \in \mathbb{C}^-} \rho[M(z)]. \tag{12}$$

The remaining parameters in the iteration matrix were chosen to force one eigenvalue of M to be zero.

In Section 3, we minimize a lower bound $f(z)$ for the spectral radius of the iteration Matrix M in regions in z plane . This bound depends only on λ, c and σ which are defined in Section 3. For the two-stage Gauss method λ, c and σ are obtained by considering the minimization problem

$$\epsilon = \min_{\lambda,\ c,\ \sigma} \sup_{z \in X} |f(z)|, \tag{13}$$

where $X \subseteq \mathbb{C}^-$. Two new schemes are proposed by considering the cases $X = \mathbb{C}^-$ and $X = \mathbb{R}^-$, where $\mathbb{R}^- = \{x \in \mathbb{R} : x \leq 0\}$. In Section 4, some numerical experiments are reported in order to confirm the results obtained in Section 3.

3. A Lower Bound for the Spectral Radius of $M(z)$

Cooper and Vignesvaran [10] restricted the iteration matrix M so that it has only one non-zero eigenvalue. In this section , this restriction is removed and a lower bound for $\rho[M(z)]$ is obtained. This lower bound depends only on λ and other two parameters. Let $\phi_1, \phi_2, \ldots, \phi_s$ be the eigenvalues of the matrix $M(z)$ given by (10). Then

$$\begin{aligned}(1-\phi_1)(1-\phi_2)\cdots(1-\phi_s)) &= \det[I_s - M(z)] \\ &= \det[P(z)]\ \det[Q(z)]. \end{aligned} \tag{14}$$

Suppose that the eigenvalues of the real matrix A are $\mu_1, \bar{\mu}_1, \mu_2, \bar{\mu}_2, \ldots,$ where $\bar{\mu}_i$ denotes the complex conjugate of $\mu_i, \quad i = 1, 2, \cdots$.
Set $\xi = \lambda z$ and $\nu_i = \dfrac{\mu_i}{\lambda}$, then the equation (14) becomes

$$(1-\phi_1)(1-\phi_2)\cdots(1-\phi_s)) = q(\xi), \tag{15}$$

where $q(\xi) = \dfrac{c(1-\sigma\xi)(1-\xi\nu_1)(1-\xi\bar{\nu}_1), \cdots, (1-\xi\nu_s)(1-\xi\bar{\nu}_s)}{(1-\xi)^{s+1}}$,

$$c = \beta(1 + (u+v)^T\eta), \quad \sigma = \frac{1 + u^T\eta}{1 + (u+v)^T\eta}. \tag{16}$$

Cooper and Vignesvaran [10] assumed that $1 \geq |\phi_1| \geq |\phi_2| \geq \cdots \geq |\phi_s|$ and derived the inequality

$$|\phi_1| \geq |1 - |q(\xi)|^{\frac{1}{s}}| \tag{17}$$

with the minimum attained if and only if $\phi_1, \phi_2, \ldots, \phi_s$ are real and equal. Now, consider the minimization problem

$$\epsilon = \min_{q} \max_{\xi \in X} |1 - |q(\xi)|^{\frac{1}{s}}|. \tag{18}$$

For given methods the coefficients of q depends on λ, σ and c only and these parameters have to be chosen to minimize the maximum of
$|1 - |q(\xi)|^{\frac{1}{s}}|$ on X. In this paper, the minimization problem (18) is solved for the two stage Gauss method for the cases $X = \mathbb{C}^-$ and $X = \mathbb{R}^-$.

3.1. The Two Stage Gauss Method

Now we restrict attention to the two-stage Gauss method. In this case, the coefficient matrix

$$A = \begin{bmatrix} a & a-b \\ a+b & a \end{bmatrix}, \quad a = \frac{1}{4}, \quad b = \frac{\sqrt{3}}{6}$$

has two distinct eigenvalues μ and $\bar{\mu}$, where $\mu = a + i\sqrt{b^2 - a^2}$. The corresponding eigenvectors are columns of the matrix

$$W = \begin{bmatrix} 1 & 1 \\ w & \bar{w} \end{bmatrix},$$

where $w = u_1 + i\ v_1, \quad v_1 \neq 0.$

Let

$$R_{12} = \eta = \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}, \quad B_{21} = u^T = \begin{pmatrix} u_1 & u_2 \end{pmatrix}, \quad L_{11} = \begin{pmatrix} 0 & 0 \\ l_1 & 0 \end{pmatrix},$$

$$L_{21} = \begin{pmatrix} l_2 & l_3 \end{pmatrix}, \quad B_{11} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix},$$

and let

$$\overline{(\eta v^T)} = W^{-1}(\eta v^T)W, \ \overline{(\eta u^T)} = W^{-1}(\eta u^T)W, \ \bar{A} = W^{-1}AW, \ \bar{B}_{11} = W^{-1}B_{11}W,$$

and $\bar{L}_{11} = W^{-1}L_{11}W$. Then

$$\bar{B}_{11} = \begin{bmatrix} \alpha & \gamma \\ \bar{\gamma} & \bar{\alpha} \end{bmatrix}, \quad \bar{L}_{11} = l \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}, \quad \bar{A} = \begin{bmatrix} \mu & 0 \\ 0 & \bar{\mu} \end{bmatrix},$$

$$\overline{(\eta v^T)} = \begin{bmatrix} \tau_1 & \theta_1 \\ \bar{\theta}_1 & \bar{\tau}_1 \end{bmatrix}, \quad \overline{(\eta u^T)} = \begin{bmatrix} \tau_2 & \theta_2 \\ \bar{\theta}_2 & \bar{\tau}_2 \end{bmatrix},$$

where

$$\tau_1 = \frac{\bar{w}r_1(l_2 - u_2l_1) - r_2(l_2 - u_2l_1) + w\bar{w}r_1l_3 - wr_2l_3}{\bar{w} - w},$$

$$\tau_2 = \frac{\bar{w}r_1u_1 + w\bar{w}r_1u_2 - r_2u_1 + wr_2u_2}{\bar{w} - w},$$

$$\theta_1 = \frac{\bar{w}r_1(l_2 - u_2l_1) - r_2(l_2 - u_2l_1) + \bar{w}^2r_1l_3 - \bar{w}r_2l_3}{\bar{w} - w},$$

$$\theta_2 = \frac{\bar{w}r_1u_1 + \bar{w}^2r_1u_2 - r_2u_1 - \bar{w}r_2u_2}{\bar{w} - w},$$

$$\alpha = \frac{\bar{w}b_{11} - b_{21} + w\bar{w}b_{12} - wb_{22}}{\bar{w} - w},$$
$$\gamma = \tfrac{\bar{w}b_{11} - b_{21} + \bar{w}^2 b_{12} - \bar{w}b_{22}}{\bar{w} - w}, \quad l = \tfrac{l_1}{\bar{w} - w}.$$

Applying these transformations into (10), we obtain

$$\bar{M}(z) = W^{-1}M(z)W$$
$$= I_2 - \frac{[(1-\lambda z)I_2 + \overline{(\eta v^T)} + (1-\lambda z)\overline{(\eta u^T)}][((1-\lambda z)I_2 + \bar{L}_{11})\bar{B}_{11}(I_2 - z\bar{A})]}{(1-\lambda z)^3},$$

and it follows that

$$\bar{M}(\xi) = \begin{bmatrix} \bar{m}_{11}(\xi) & \bar{m}_{12}(\xi) \\ \bar{m}_{21}(\xi) & \bar{m}_{22}(\xi) \end{bmatrix}$$

where $\xi = \lambda z$, $\nu = \frac{\mu}{\lambda}$, $\psi = \alpha - (\alpha + \bar{\gamma})l$, $\chi = \gamma - (\gamma + \bar{\alpha})l$,

$$\bar{m}_{11}(\xi) = 1 - \tfrac{(1-\xi\nu)[(1-\xi+\tau_1+(1-\xi)\tau_2)(\psi-\alpha\xi)+(\theta_1+(1-\xi)\theta_2)(\bar{\chi}-\bar{\gamma}\xi)]}{(1-\xi)^3},$$

$$\bar{m}_{12}(\xi) = -\tfrac{(1-\xi\bar{\nu})[(1-\xi+\tau_1+(1-\xi)\tau_2)(\chi-\gamma\xi)+(\theta_1+(1-\xi)\theta_2)(\bar{\psi}-\bar{\alpha}\xi)]}{(1-\xi)^3},$$

$$\bar{m}_{21}(\xi) = -\tfrac{(1-\xi\nu)[(\bar{\theta}_1+(1-\xi)\bar{\theta}_2)(\psi-\alpha\xi)+(1-\xi+\bar{\tau}_1+(1-\xi)\bar{\tau}_2)(\bar{\chi}-\bar{\gamma}\xi)]}{(1-\xi)^3},$$

$$\bar{m}_{22}(\xi) = 1 - \tfrac{(1-\xi\bar{\nu})[(\bar{\theta}_1+(1-\xi)\bar{\theta}_2)(\chi-\gamma\xi)+(1-\xi+\bar{\tau}_1+(1-\xi)\bar{\tau}_2)(\bar{\psi}-\bar{\alpha}\xi)]}{(1-\xi)^3}.$$

The eigenvalues ϕ_1 and ϕ_2 of $\bar{M}(\xi)$ are solutions of

$$\phi^2 - p(\xi)\ \phi + p(\xi) - 1 + q(\xi) = 0, \tag{19}$$

where

$$p(\xi) = 2 - \frac{(1-\xi\nu)[(1-\xi+\tau_1+(1-\xi)\tau_2)(\psi-\alpha\xi)+(\theta_1+(1-\xi)\theta_2)(\bar{\chi}-\bar{\gamma}\xi)]}{(1-\xi)^3}$$
$$- \frac{(1-\xi\bar{\nu})[(\bar{\theta}_1+(1-\xi)\bar{\theta}_2)(\chi-\gamma\xi)+(1-\xi+\bar{\tau}_1+(1-\xi)\bar{\tau}_2)(\bar{\psi}-\bar{\alpha}\xi)]}{(1-\xi)^3},$$

$$q(\xi) = \frac{c(1-\sigma\xi)(1-\xi\nu)(1-\xi\bar{\nu})}{(1-\xi)^3}. \tag{20}$$

From (17), $|\phi_1| \geq |1 - |q(\xi)|^{\frac{1}{2}}|$ with the minimum attained if and only if ϕ_1 and ϕ_2 are real and equal. That is, $|\phi_1| = |1 - |q(\xi)|^{\frac{1}{2}}|$ if and only if

$$\left(\frac{p(\xi)}{2} - 1\right)^2 = q(\xi). \tag{21}$$

Let $X = \mathbb{C}^-$. To find $|\epsilon| = \min_q \max_{\xi \in \mathbb{C}^-} |1 - |q(\xi)|^{\frac{1}{2}}|$, observe that $q(\xi)$ is analytic and bounded on $\mathbb{C}^-$ and hence $|1 - |q(\xi)|^{\frac{1}{2}}|$ attains its maximum on the imaginary axis $\xi = i\ y$, $y \in \mathbb{R}$. Let $r(\omega) = 1 - |q(iy)|^{\frac{1}{2}}$, where $\omega = \dfrac{1}{1+y^2}$. It follows that

$$r(\omega) = 1 - [a_0\omega^3 + a_1\omega^2(1-\omega) + a_2\omega(1-\omega)^2 + a_3(1-\omega)^3]^{\frac{1}{4}}$$

where

$$a_0 = c^2, \quad a_1 = c^2((\sigma+\nu+\bar{\nu})^2 - 2(\nu\bar{\nu} + \sigma(\nu+\bar{\nu}))),$$
$$a_2 = c^2((\nu\bar{\nu} + \sigma(\nu+\bar{\nu}))^2 - 2\sigma\nu\bar{\nu}(\sigma+\nu+\bar{\nu})), \quad a_3 = (c\sigma\nu\bar{\nu})^2.$$

These coefficients depend on λ, σ and c only and these parameters have to be chosen to minimize the maximum of $|r(\omega)|$ on $[0,1]$. The maximum of $|r(\omega)|$ occurs at the end points of $[0,1]$ or at

$$\omega_1 = \frac{-(a_1 - 2a_2 + 3a_3) + ((a_1 - 2a_2 + 3a_3)^2 - 3(a_0 - a_1 + a_2 - a_3)(a_2 - 3a_3))^{\frac{1}{2}}}{3(a_0 - a_1 + a_2 - a_3)},$$

or at

$$\omega_2 = \frac{-(a_1 - 2a_2 + 3a_3) - ((a_1 - 2a_2 + 3a_3)^2 - 3(a_0 - a_1 + a_2 - a_3)(a_2 - 3a_3))^{\frac{1}{2}}}{3(a_0 - a_1 + a_2 - a_3)},$$

where $\dfrac{d}{d\omega}[r(\omega)] = 0$ at $\omega = \omega_1$ and $\omega = \omega_2$.
Since $r(\omega)$ is continuous on $[0,1]$, λ, σ and c must be chosen so that $r(\omega)$ equioscillates four times on [0,1]. Hence $r(0) = r(\omega_2) = \epsilon$ and $r(1) = r(\omega_1) = -\epsilon$. This gives $\lambda = 0.217129273$ $, c = 1.027954404$ $, \sigma = 0.535183758$, and $\epsilon = 0.0139$, and this occurs when $\xi = 0,\ \pm\sqrt{3}i,\ \pm\frac{i}{\sqrt{3}},\ \pm\infty$. For these values of ξ, the equation (21) holds. This gives

$$\begin{aligned}
\zeta^2 &= 4c, \\
((\zeta - 3\kappa_2) \pm i\sqrt{3}(\kappa_1 - 3\vartheta))^2 &= 4c(\delta_1 \pm i\sqrt{3}\varsigma_1), \\
((\zeta - \frac{1}{3}\kappa_2) \pm i\frac{1}{\sqrt{3}}(\kappa_1 - \frac{1}{3}\vartheta))^2 &= 4c(\delta_2 \pm i\frac{1}{\sqrt{3}}\varsigma_2), \\
\vartheta^2 &= 4c\sigma|\nu|^2,
\end{aligned}$$

where $\zeta = 2\ \mathrm{Re}(\psi(1+\tau_1+\tau_2) + \bar{\chi}(\theta_1+\theta_2))$, $\vartheta = 2\ \mathrm{Re}(\nu(\alpha(1+\tau_2) + \bar{\gamma}\theta_2))$, $\kappa_1 = 2\ \mathrm{Re}(\alpha(1+\tau_1+\tau_2) + \psi + \nu\psi(1+\tau_1+\tau_2) + \tau_2\psi + \bar{\gamma}(\theta_1+\theta_2) + \chi\bar{\theta}_2 + \chi\bar{\nu}(\bar{\theta}_1 + \bar{\theta}_2))$, $\kappa_2 = 2\ \mathrm{Re}(\alpha + \alpha\nu(1+\tau_1+\tau_2) + \alpha\tau_2 + \nu\psi(1+\tau_2) + \theta_2\bar{\gamma} + \nu\bar{\gamma}(\theta_1+\theta_2) +$

$\bar{\nu}\chi\bar{\theta}_2)$, $\delta_1 = 8(3\sigma\nu + 3\sigma\bar{\nu} + 3\nu\bar{\nu} - 1)$, $\varsigma_1 = 8(3\sigma\nu\bar{\nu} - (\sigma + \nu + \bar{\nu}))$, $\delta_2 = \frac{8}{27}(\sigma\nu\bar{\nu} - 3(\sigma + \nu + \bar{\nu}))$, $\varsigma_2 = \frac{8}{9}(3 - \sigma\nu - \sigma\bar{\nu} - \nu\bar{\nu})$.

This implies

$$\begin{aligned}
\zeta^2 &= 4c, \\
(\zeta - 3\kappa_2)^2 - 3(\kappa_1 - 3\vartheta)^2 &= 4c\delta_1, \\
(\zeta - 3\kappa_2)(\kappa_1 - 3\vartheta) &= 2c\varsigma_1, \\
(\zeta - \frac{1}{3}\kappa_2)^2 - \frac{1}{3}(\kappa_1 - \frac{1}{3}\vartheta)^2 &= 4c\delta_2, \\
(\zeta - \frac{1}{3}\kappa_2)(\kappa_1 - \frac{1}{3}\vartheta) &= 2c\varsigma_2, \\
\vartheta^2 &= 4c\sigma|\nu|^2.
\end{aligned}$$

These six conditions and the equations (16) give eight equations in eleven unknown elements of the parameter matrices. These equations may be solved by choosing $B_{21} = 0$ and B_{11} as lower triangular matrix. Hence, we obtain

$$\begin{aligned}
S &= I_2, \quad L_{21} = [-1.211288546 \quad 0.863683808], \\
R_{12}^T &= [-0.171698521 \quad 0.764794515], \\
B_{11} &= \begin{bmatrix} 1.214917992 & 0 \\ -0.292049833 & 0.452824393 \end{bmatrix}, \\
L_{11} &= \begin{bmatrix} 0 & 0 \\ 1.304771023 & 0 \end{bmatrix},
\end{aligned} \tag{22}$$

and the corresponding eigenvalues of $\bar{M}$ are given by

$$\phi(\xi) = \frac{p(\xi) \pm \sqrt{(p(\xi))^2 - 4(p(\xi) - 1 + q(\xi))}}{2}.$$

With the parameters given by (22), we obtain $\rho[\bar{M}(\xi)] \leq 0.0256$ for all $\xi \in \mathbb{C}^-$ with lower bound $|\epsilon| = 0.0139$ attained at $\xi = 0, \ \pm\sqrt{3}i, \ \pm\frac{i}{\sqrt{3}}, \ \pm\infty$ and is exceeded elsewhere in the imaginary axis $\xi = iy$. This result is appreciably better than the result obtained in [10].

3.2. Minimization on the Negative Real Axis

In this case $|1-|q(\xi)|^{\frac{1}{2}}|$ attains its maximum on the negative real axis $\xi = x,\ x \in \mathbb{R}^-$. Let $r_1(\omega) = 1-|q(x)|^{\frac{1}{2}}$, where $\omega = \dfrac{1}{1-x}$. It follows that

$$r_1(\omega) = 1 - [b_0\omega^3 + b_1\omega^2(1-\omega) + b_2\omega(1-\omega)^2 + b_3(1-\omega)^3]^{\frac{1}{2}}$$

where

$$b_0 = c, \quad b_1 = c(\sigma+\nu+\bar{\nu}),$$
$$b_2 = c(\nu\bar{\nu} + \sigma(\nu+\bar{\nu})), \quad b_3 = (c\sigma\nu\bar{\nu}).$$

These coefficients depend on λ, σ and c only and these parameters have to be chosen to minimize the maximum of $|r_1(\omega)|$ on $[0,1]$. The maximum of $|r_1(\omega)|$ occurs at the end points of $[0,1]$ or at

$$\omega_1 = \frac{-(b_1-2b_2+3b_3) + ((b_1-2b_2+3b_3)^2 - 3(b_0-b_1+b_2-b_3)(b_2-3b_3))^{\frac{1}{2}}}{3(b_0-b_1+b_2-b_3)}$$

or at

$$\omega_2 = \frac{-(b_1-2b_2+3b_3) - ((b_1-2b_2+3b_3)^2 - 3(b_0-b_1+b_2-b_3)(b_2-3b_3))^{\frac{1}{2}}}{3(b_0-b_1+b_2-b_3)},$$

where $\dfrac{d}{d\omega}[r_1(\omega)] = 0$ at $\omega = \omega_1$ and $\omega = \omega_2$.
Since $r_1(\omega)$ is continuous on $[0,1]$, λ, σ and c must be chosen so that $r_1(\omega)$ equioscillates four times on [0,1]. Hence $r_1(0) = r_1(\omega_2) = \epsilon$ and $r_1(1) = r_1(\omega_1) = -\epsilon$. This gives $\lambda = 0.388797743\ \ , c = 0.993103367\ \ , \sigma = 1.839202054$ and $\epsilon = 0.0035$, and this occurs when $\xi = 0,\ -3,\ -\frac{1}{3},\ -\infty$. For these values of ξ, equation (21) holds. This gives

$$\begin{aligned} \zeta^2 &= 4c, \\ (\zeta - 3\kappa_1 + 9\kappa_2 - 27\vartheta)^2 &= 4c\delta, \\ (\zeta - \frac{1}{3}\kappa_1 + \frac{1}{9}\kappa_2 - \frac{1}{27}\vartheta)^2 &= 4c\varsigma, \\ \vartheta^2 &= 4c\sigma|\nu|^2, \end{aligned}$$

where $\zeta = 2\ \mathrm{Re}(\psi(1+\tau_1+\tau_2) + \bar{\chi}(\theta_1+\theta_2)), \quad \vartheta = 2\ \mathrm{Re}(\nu(\alpha(1+\tau_2) + \bar{\gamma}\theta_2))$, $\kappa_1 = 2\ \mathrm{Re}(\alpha(1+\tau_1+\tau_2) + \psi + \nu\psi(1+\tau_1+\tau_2) + \tau_2\psi + \bar{\gamma}(\theta_1+\theta_2) + \chi\bar{\theta}_2 + \chi\bar{\nu}(\bar{\theta}_1 +$

$\bar{\theta}_2)),\ \ \kappa_2 = 2\ \mathrm{Re}(\alpha + \alpha\nu(1+\tau_1+\tau_2) + \alpha\tau_2 + \nu\psi(1+\tau_2) + \theta_2\bar{\gamma} + \nu\bar{\gamma}(\theta_1+\theta_2) + \bar{\nu}\chi\bar{\theta}_2),\quad \delta = 64(1 + 3(\sigma+\nu+\bar{\nu}) + 9\sigma\nu + 9\sigma\bar{\nu} + 9\nu\bar{\nu} + 27\sigma\nu\bar{\nu}),$
$\varsigma = \frac{64}{729}(27 + 9(\sigma+\nu+\bar{\nu}) + 3\sigma\nu + 3\sigma\bar{\nu} + 3\nu\bar{\nu} + \sigma\nu\bar{\nu}).$

These four conditions and the equations (16) give various schemes. One particular scheme is obtained by choosing $B_{21} = 0,\ R_{12}^T = [1,1]$ and the first element of L_{21} as zero. Hence, we obtain

$$\begin{aligned} S &= I_2, \quad L_{21} = [0 \quad -0.456285949], \\ B_{11} &= \begin{bmatrix} 1.745600824 & 0.134428143 \\ -0.508658139 & 1.007183177 \end{bmatrix}, \\ L_{11} &= \begin{bmatrix} 0 & 0 \\ 0.735721095 & 0 \end{bmatrix}, \end{aligned} \tag{23}$$

and the corresponding eigenvalues of $\bar{M}$ is given by

$$\phi(\xi) = \frac{p(\xi) \pm \sqrt{(p(\xi))^2 - 4(p(\xi) - 1 + q(\xi))}}{2}.$$

It follows from (23) that $\rho[\bar{M}(\xi)] = 0.0035$ for all $\xi \in \mathbb{R}^-$ and this gives the scheme an advantage though in general $\rho[\bar{M}(\xi)] \leq 0.0385$ for all $\xi \in \mathbb{C}^-$.

4. Numerical Results

A variety of numerical experiments was carried out in order to evaluate the efficiency of the schemes obtained here. For each experiment, a single step was carried out, in each case, using the Jacobian evaluated at the initial point. For each scheme tested, the initial iterate Y^0 is chosen as $Y^0 = x \oplus x \oplus \cdots \oplus x$, where x is the true solution at the initial point. Results for seven non-linear initial value problems are reported and compared with results obtained using the schemes described in [8], [10].

Problem 1 denotes the non-linear system given by [14]

$$\begin{aligned} x_1' &= -0.013x_1 + 1000x_1x_3, & x_1(0) &= 1, \\ x_2' &= 2500x_2x_3, & x_2(0) &= 1, \\ x_3' &= 0.013x_1 - 1000x_1x_3 - 2500x_2x_3, & x_3(0) &= 0, \end{aligned}$$

where the eigenvalues of the Jacobian at the initial point are 0, -0.0093 and -3500.

Problem 2 is also the non-linear system, also given by [14],

$$\begin{aligned} x_1' &= -55x_1 + 65x_2 - x_1x_3, & x_1(0) &= 1, \\ x_2' &= 0.0785(x_1 - x_2),, & x_2(0) &= 1, \\ x_3' &= 0.1x_1, & x_3(0) &= 0, \end{aligned}$$

where , initially,the eigenvalues of the Jacobian are the complex conjugate pair $-0.0062 \pm 0.01i$ and -55.

Problem 3 Insulator physics: Klopfenstein (1970),

$$\begin{aligned} x_1' &= -x_1 + 10^8 x_3(1 - x_1), & x_1(0) &= 1, \\ x_2' &= -10x_2 + 3 \times 10^7 x_3(1 - x_2), & x_2(0) &= 0, \\ x_3' &= -x_1' - x_2', & x_3(0) &= 0, \end{aligned}$$

where the eigenvalues are 0, -1.0 and -3.0×10^7.

Problem 4 is the HIRES problem given by [19],

$$\begin{aligned} x_1' &= -x_1 + 2, & x_1(0) &= 1, \\ x_2' &= -10x_2 + 0.1x_1^2, & x_2(0) &= 1, \\ x_3' &= -40x_3 + 0.4\left(x_1^2 + x_2^2\right), & x_3(0) &= 1, \\ x_4' &= -100x_4 + x_1^2 + x_2^2 + x_3^2, & x_4(0) &= 1, \end{aligned}$$

where the Jacobian has constant eigenvalues -1, -10, -40 and -100.

Problem 5 is the elliptic two-body problem, with eccentricity 0.6,

$$\begin{aligned} x_1' &= x_3, & x_1(0) &= 0.4, \\ x_2' &= x_4, & x_2(0) &= 0, \\ x_3' &= -x_1\left(x_1^2 + x_2^2\right)^{-3/2}, & x_3(0) &= 0, \\ x_4' &= -x_2\left(x_1^2 + x_2^2\right)^{-3/2}, & x_4(0) &= 2. \end{aligned}$$

The eigenvalues at the initial point are ± 5.5902 and $\pm 3.9528i$.

Problem 6 Chemistry: Bjurel et. al.[15],

$$\begin{aligned} x_1' &= x_3 - 100x_1x_2, & x_1(0) &= 1, \\ x_2' &= x_3 + 2x_4 - 100x_1x_2 - 2 \times 10^4 x_2^2, & x_2(0) &= 1, \\ x_3' &= -x_3 + 100x_1x_2, & x_3(0) &= 0, \\ x_4' &= -x_4 + 10^4 x_2^2, & x_3(0) &= 0, \end{aligned}$$

where the eigenvalues are $0, -0.002$, -100 and -4.0×10^4.

Problem 7 denotes the system, with non-linear coupling between smooth and transient components,

$$\begin{aligned} x_1' &= -10^5 x_1 + 2, & x_1(0) &= 1, \\ x_2' &= -10^6 x_2 + 0.1 x_1^2, & x_2(0) &= 1, \\ x_3' &= -40 \times 10^5 x_3 + 0.4\left(x_1^2 + x_2^2\right), & x_3(0) &= 1, \\ x_4' &= -10^7 x_4 + x_1^2 + x_2^2 + x_3^2, & x_4(0) &= 1, \end{aligned}$$

where the Jacobian has constant eigenvalues -10^5, -10^6, -40×10^5 and -10^7.

Method 1 denotes the two-stage Gauss method implemented according to the basic scheme (6) with parameters given in [8, p.138].
Method 2 is the same Gauss method implemented using the scheme (7) with one extra sub-step $r = s + 1$ and with parameters given in [10, p.221].
Method 3 is the same Runge-Kutta method implemented according to the scheme (7) with $r = s + 1$ and with parameters $\lambda = 0.217129273$ $, c = 1.027954404$ $, \sigma = 0.535183758$, and other parameter matrices given by (22).
Method 4 is the same Gauss method implemented using the scheme (7) with $r = s + 1$ and with parameters $\lambda = 0.388797743$, $c = 0.993103367$, $\sigma = 1.839202054$ and other parameter matrices given by (23).

For each method and problem, the quantities

$$e_m = \|E^m\|, \quad m = 1, 2, 3, \cdots$$

were computed using the maximum norm on $\mathbb{R}^{ns}$. The values m for which $e_m \leq$ TOL $= 10^{-9}$ are tabulated for each problem and method in Table 1. The detailed results for e_m for all problems are give in Tables 2 - 8. Similar results are obtained for different values of TOL and these are not reported here.

The numerical results shows that the new methods 3 and 4 perform better than the methods 1 and 2. The method 4 is marginally better than the method 3. In overall, the best performance was obtained in Method 4 since $\rho[\bar{M}(0)]$ is smallest in this case.

Problem	h	Method 1	Method 2	Method 3	Method 4
1	0.1	7	6	5	5
2	1.0	8	7	7	6
3	3.3×10^{-4}	6	6	5	5
4	0.01	8	7	6	6
5	0.01	8	7	6	6
6	2.5×10^{-7}	8	6	5	5
7	0.1	9	8	7	6

Table 1: Values of m giving $e_m \leq 10^{-9}$ for two-stage Gauss method

Method 1	Method 2	Method 3	Method 4
0.000785721	0.000753411	0.000752338	0.000524945
0.000056476	0.000313924	0.000019405	0.000209617
0.000004034	0.000008559	0.000000417	0.000001509
0.000000287	0.000000213	0.000000022	0.000000008
0.000000020	0.000000005	0.000000000	0.000000000
0.000000001	0.000000000		
0.000000000			

Table 2: Detailed Results for Problem 1

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Method 1	Method 2	Method 3	Method 4
0.213924116	0.199557474	0.257850381	0.314768463
0.012551776	0.040314932	0.054786238	0.112829333
0.000768439	0.001146766	0.000994130	0.000192104
0.000047528	0.000034870	0.000025059	0.000084464
0.000002979	0.000001091	0.000000983	0.000000032
0.000000210	0.000000034	0.000000002	0.000000001
0.000000015	0.000000001	0.000000001	0.000000000
0.000000001	0.000000000		
0.000000000			

Table 3: Detailed Results for Problem 2

Method 1	Method 2	Method 3	Method 4
0.000278905	0.000267449	0.000266923	0.000185918
0.000020157	0.000111532	0.000006951	0.000073779
0.000001467	0.000003192	0.000000135	0.000000443
0.000000107	0.000000107	0.000000009	0.000000003
0.000000008	0.000000004	0.000000000	0.000000000
0.000000001	0.000000000		

Table 4: Detailed Results for Problem 3

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Method 1	Method 2	Method 3	Method 4
0.548286660	0.540353196	0.547959036	0.441135662
0.021941662	0.176368772	0.011786571	0.095735108
0.000717959	0.001684179	0.000074898	0.000742853
0.000032637	0.000045684	0.000005413	0.000025290
0.000001487	0.000000725	0.000000046	0.000000308
0.000000091	0.000000013	0.000000001	0.000000001
0.000000006	0.000000000		
0.000000000			

Table 5: Detailed Results for Problem 4

Method 1	Method 2	Method 3	Method 4
0.052862432	0.050684222	0.050583566	0.035209143
0.003864295	0.021174600	0.001329989	0.013988848
0.000289735	0.000650475	0.000013504	0.000096073
0.000021721	0.000032360	0.000000622	0.000008801
0.000001632	0.000001143	0.000000035	0.000000142
0.000000123	0.000000039	0.000000001	0.000000001
0.000000009	0.000000001	0.000000000	0.000000000
0.000000001	0.000000000		

Table 6: Detailed Results for Problem 5

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Method 1	Method 2	Method 3	Method 4
0.040545482	0.004055616	0.004048240	0.002825693
0.002746538	0.001685355	0.000102755	0.001114616
0.000173209	0.000046141	0.000002043	0.000007146
0.000010785	0.000001257	0.000000037	0.000000038
0.000000672	0.000000034	0.000000001	0.000000000
0.000000042	0.000000001		
0.000000003			
0.000000000			

Table 7: Detailed Results for Problem 6

Method 1	Method 2	Method 3	Method 4
1.072046808	0.972637267	1.360544425	1.766591394
0.076951067	0.241481908	0.350339676	0.771872605
0.005524848	0.006702290	0.009987571	0.005311999
0.000396665	0.000186022	0.000209748	0.000027455
0.000028479	0.000005163	0.000003898	0.000000126
0.000002045	0.000000143	0.000000068	0.000000001
0.000000147	0.000000004	0.000000001	
0.000000011	0.000000000		
0.000000001			

Table 8: Detailed Results for Problem 7

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