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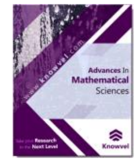

Original Research Article

A Class of S-step Non-Linear Iteration Scheme Based on Projection Method for Gauss Method

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Abstract

Various iteration schemes are proposed by various authors to solve non-linear equations arising in the implementation of implicit Runge-Kutta methods. In this paper, a class of s-step non-linear scheme based on projection method is proposed to accelerate the convergence rate of those linear iteration schemes. In this scheme, sequence of numerical solutions is updated after each sub-step is completed. For 2-stage Gauss method, upper bound for the spectral radius of its iteration matrix was obtained in the left half complex plane. This result is extended to 3-stage and 4-stage Gauss methods by transforming the coefficient matrix and the iteration matrix to a block diagonal form. Finally, some numerical experiments are carried out to confirm the obtained theoretical results.

Keywords: Gauss method, implementation, projection method, rate of convergence, stiff systems

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1. Introduction

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

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

An s-stage implicit Runge-Kutta method computes an approximation x_{r+1} to the solution $x(t_{r+1})$ at discrete 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 $y_1, y_2, \ldots, y_s$ satisfy *Sn* equations

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

and $A = \left[a_{ij}\right]$ is the real coefficient matrix 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 the equations (2) written by $D(Y) = 0,$ where D is the approximation defect defined by

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

Where $e = (1,1,\ldots,1)^T$ and $A \otimes I_n$ is the tensor product of the matrix A with $n \times n$ identity matrix I_n and, in general $A \otimes B = [a_{ij}B]$. This article deals with methods suitable for stiff systems so that the matrix A is not strictly lower triangular. There are two general approaches proposed by several authors to solve the system $D(Y) = 0$. In one approach, a modified Newton scheme is used. 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

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

In each step of this iteration, a set of *sn* linear equations has to be solved so that this scheme is still expensive. The other approach is to use schemes based directly on iterative procedures. In this type, several authors proposed several iteration schemes. A more general scheme was proposed by Cooper and Butcher [1]. This scheme sacrificing super linear convergence for reduced linear algebra cost. They consider the scheme

$$\left[I_s\otimes\left(I_n-h\lambda J\right)\right]E^m=\left(BS^{-1}\otimes I_n\right)D\left(Y^{m-1}\right)+\left(L\otimes I_n\right)E^m,$$
$$Y^m=Y^{m-1}+\left(S\otimes I_n\right)E^m,\quad m=1,2,\ldots,\qquad (5)$$

Where *B* and *S* are real $s\times s$ non-singular matrices and *L* is strictly lower triangular matrix of order *s,* and λ is a real constant. Cooper and Butcher [1] also showed that successive over-relaxation may be applied to improve the rate of convergence for scalar test problem. Cooper and Vigneswaran [2] proposed an efficient scheme where the elements $Y^m=y_1^m\oplus y_2^m\oplus\cdots\oplus y_s^m$ are obtained in sequence and the approximation defect is updated after each sub-step is completed. Only one vector transformation is needed for each full step. The rate of convergence of this scheme has been improved in [3], [4], and [5]. Cooper and Vigneswaran [6] proposed another scheme, which is a generalization of the basic scheme (5), to obtain improved rate of convergence, by adding extra sub- steps. Further improvement in the rate of convergence of this scheme has been obtained in [7].

In this paper, in order to accelerate the convergence rate of the proposed linear iteration schemes Vigneswaran [8] proposed a class of non-linear iteration scheme based on projection method. This scheme is discussed detail in the section 2. In section 3, this result is extended to the higher order Gauss methods such as three-stage and four-stage. In the final section numerical results are carried out to confirm the obtained results.

2. A CLASS OF NON-LINEAR SCHEMES BASED ON PROJECTION METHOD

2.1 Projection method for linear system

More attention have been taken on Jacobi and the Gauss-Seidel schemes and their accelerated forms when solving large linear algebraic systems of equations. But Householder [9] proposed a class of method with the help of functional analysis approach which has been called projection method. This techniques have been used to accelerate convergence of iterative process for non-linear problems.

Consider solving the linear system $Ax=b,$ where *A* is assumed to be a $n\times n$ non-singular matrix. Let x_k represent any iterate and let $\delta_k=x-x_k,\ r_k=b-Ax_k,$ represent the error and residual respectively, where *x* is the true solution. A method of projection is one in which at each step, the error δ_k is resolved into two components, one of which is required to lie in a subspace selected at that step, and the other is $\delta_{k+1},$ which is required to be less than δ_k in some norm. The subspace is selected by choosing a matrix Y_k, whose columns are linearly independent and form a basis for the subspace. In practice Y_k is generally a single vector y_k. That is, $\delta_{k+1}=\delta_k-Y_ku_k,$ where u_k is a vector (or scalar if Y_k is a vector) to be selected at the k^{th} step so that $\delta_{k+1}\le\delta_k$. Householder shows that δ_{k+1} is minimized by choosing u_k so that Y_ku_k is the projection of δ_k onto the subspace spanned by the columns of Y_k with respect to *G*, where *G* is a positive definite matrix. This implies that δ_{k+1} is minimized when $Y_k^HG\left(\delta_k-Y_ku_k\right)=0,$ where $Y_k^H=\bar{Y}_k^T$ is the Hermitian of Y_k. Here $\|\cdot\|$ is defined by $\|\delta_k\|^2=\delta_k^HG\delta_k$.

2.2 A class of non-linear scheme

The above idea is used to solve the non-linear system of equations $D(Y)=0.$ Vigneswaran [8] proposed a non-linear scheme based on projection method is of the form

$$Y^{m+1}=Y^m+\mu^mE^m,\ m=1,2,3,\ldots,\qquad (6)$$

Where μ^m is scalar and E^m is a vector. Let $\Delta^m=Y-Y^m$. In this new scheme, E^m is chosen from the general linear iteration scheme. The scalar μ^m is chosen as μ^mE^m is the projection Δ^m onto E^m with respect to a positive definite matrix $G^HG,$ where G is a $sn\times sn$ non-singular matrix. Hence

$$\Delta^{m+1}=\Delta^m-\mu^mE^m,$$

$$\mu^m=\frac{\left(GE^m\right)^H G\Delta^m}{\left(GE^m\right)^H\left(GE^m\right)},\ m=1,2,3,\ldots.\qquad (7)$$

Suppose that the sequence $Y^m\to Y$ as $m\to\infty.$ if E^m is chosen so that $E^m\to 0$ gives $D\left(Y^m\right)\to 0,$ it follows that $D(Y)=0.$ Here *G* and E^m have to be chosen so that the scheme can be efficiently implemented and performs well. In each step of the iteration (6) the scalar μ^m has to be calculated by using (7) but the numerator of μ^m contains Δ^m which is not known. To make the process feasible the matrix *G* may be chosen as $\left(Q\otimes I_n\right)D'\left(Y^m\right),$ where *Q* is a $s\times s$ non-singular matrix. Since $D\left(Y^m\right)=-D'\left(Y^m\right)\Delta^m+O\left(\left\|\Delta^m\right\|\right)^2,$ $G\Delta^m$ may be approximated by $\left(Q\otimes I_n\right)D\left(Y^m\right)$. Since $F'\left(Y^m\right)$ is the block diagonal matrix and each diagonal block is the Jacobian off at one of $y_1^m,y_2^m,\ldots,y_s^m$. Thus the evaluation of $D'\left(Y^m\right)$ requires more computation. To reduce this, the Jacobian is computed infrequently. Let *J* be the Jacobian evaluated at recent point x_p. then $F'\left(x_p\right)=I_s\otimes J$ and $D'\left(Y^m\right)=-\left(I_{sn}-hA\otimes J\right).$ Hence from (7), we obtain

$$\mu^m=\frac{\left[\left(Q\otimes I_n\right)\left(I_{sn}-hA\otimes J\right)E^m\right]^H\left(Q\otimes I_n\right)D\left(Y^m\right)}{\left[\left(Q\otimes I_n\right)\left(I_{sn}-hA\otimes J\right)E^m\right]^H\left[\left(Q\otimes I_n\right)\left(I_{sn}-hA\otimes J\right)E^m\right]},\qquad (8)$$

Where $E^m=E_1^m\oplus E_2^m\oplus\cdots\oplus E_s^m$ and

$E_i^m=O\oplus O\oplus\cdots\oplus O\oplus\varepsilon_i^m\oplus O\oplus\cdots\oplus O,$ *O* the zero vector.

2.2.1 The s-step non-linear scheme

Vigneswaran [8] also consider the s-step non-linear scheme which is more efficient than the general class of non-linear scheme given by (6) with (8). In this scheme elements of $Y^m = y_1^m \oplus y_2^m \oplus \cdots \oplus y_s^m$ are obtained in sequence and are updated after each sub-step is completed. He consider the scheme

$$Y^m = Y^{(1)},$$

$$\mu_i^m = \frac{\left[(Q\otimes I_n)(I_{sn} - hA\otimes J)E_i^m\right]^H (Q\otimes I_n)D\left(Y^{(i)}\right)}{\left[(Q\otimes I_n)(I_{sn} - hA\otimes J)E_i^m\right]^H \left[(Q\otimes I_n)(I_{sn} - hA\otimes J)E_i^m\right]}, \qquad (9)$$

$$Y^{(i+1)} = Y^{(i)} + \mu_i^m E_i^m, \; i = 1,2,\ldots s,$$

$$Y^{(s+1)} = Y^{m+1}, \quad m = 1,2,3,\ldots.$$

In this scheme

$$Y^{(i)} = y_1^{(m+1)} \oplus y_2^{(m+1)} \oplus \cdots \oplus y_i^{(m+1)} \oplus y_{i-1}^{(m+1)} \oplus y_{i+1}^{(m+1)} \oplus \cdots \oplus y_i^{(m)}$$

for $i = 1,2,\ldots,s.$

The non-singular matrix *Q* and E^m have to be chosen so that the scheme performs well. The efficiency of this scheme examined when it is applied to the linear scalar problem $x' = qx$ with rapid convergence required for all

$$z = hq \in \mathbb{C}^- = \{z \in \mathbb{C} \mid \mathrm{Re}(z) \le 0\}$$

This gives

$$\Delta^{m+1} = M(z)\Delta^m, \quad m = 1,2,\ldots.$$

Where the iteration matrix is given as

$$M(z) = -\left[D(z) + L(z)\right]^{-1} L^H(z), \qquad (10)$$

Where $L(z) = (l_{ij}(z))$ is a strictly lower triangular matrix and $D(z) = (l_{ii}(z))$ is a diagonal matrix and $l_{ij}(z) = e_i^H (I_s - zA)^H Q^H Q (I_s - zA) e_j,$ these elements are independent of the choice of E^m. Hence *Q* should be chosen to minimize the spectral radius of $M(z)$ over $\mathbb{C}^-$. This seems to be very difficult. We apply a different approach which is we impose spectral radius of *M (z)* to be zero for real *z*. The following theorem gives an upper bound for $\rho[M(z)]$ for the two stage Gauss method in the left half plane. The coefficient matrix of the two stage Gauss method is given by

$$A = \begin{bmatrix} a_1 & a_1 - b_1 \\ a_1 + b_1 & a_1 \end{bmatrix}, \qquad (11)$$

Where $a_1 = \frac{1}{4}$ and $b_1 = \frac{\sqrt{3}}{6}.$

Theorem 1. Consider the two-stage Gauss method with coefficient matrix given by (11) and *S = I*. Suppose that $\rho[M(z)] = 0$ on the real axis *z = x*. Then there exists a non-singular matrix *Q* such that

$$Q^H Q = \begin{pmatrix} 1 & 0 \\ 0 & \frac{b_1 - a_1}{b_1 + a_1} \end{pmatrix}$$

and

$$\rho[M(z)] \le 1 - \left(\frac{a_1}{b_1}\right)^2 \quad \text{for all } z \in \mathbb{C}^-.$$

In this approach, it is difficult to handle the 3-stage Gauss method and 4-stage Gauss method. We may transform the coefficient matrix and the iteration matrix to a block diagonal matrix. The result for *s* = 2 may be applied to other methods when *s* > 2.

3. Improved Convergence Rate for s>2

Many iterative methods have coefficient matrices which may be transformed to real block diagonal matrices.

For each *s*- stage method of order 2*s* there is a real matrix *S* such that

$$S^{-1}AS = \bar{A} = A_1 \oplus A_2 \oplus \cdots \oplus A_r \qquad (12)$$

A real block diagonal matrix. The sub matrices are chosen to have the form

$$A_i = \begin{bmatrix} a_i & a_i - b_i \\ a_i + b_i & a_i \end{bmatrix}, \quad i = 1,2,\ldots,r, \qquad (13)$$

with $b_i > a_i, \; i = 1,2,\ldots,r$ and except that, when *s* is odd $A_r = [a_r]$. Many iterative methods have coefficient matrices which may be transformed to real block diagonal matrices of the same form as (12). The iteration matrix *M (z)* can be written as a partition form corresponding to the partition of $S^{-1}AS$:

$$S^{-1}M(z)S = \bar{M}(z) = M_1(z) \oplus M_2(z) \oplus \cdots \oplus M_r(z).$$

Then the spectral radius is given by

$$\rho\left[\bar{M}(z)\right] = \max_{1\le i\le r} \rho\left[M_i(z)\right],$$

$$M_i(z) = -\left[D_i(z) + L_i(z)\right]^{-1} L_i^H(z), \quad i = 1,2,\ldots,r, \qquad (14)$$

$$D(z) = D_1(z) \oplus D_2(z) \oplus \cdots \oplus D_r(z) \quad \text{and}$$

$$L(z) = L_1(z) \oplus L_2(z) \oplus \cdots \oplus L_r(z)$$

Corresponding to the partition of $S^{-1}AS$. When *s* = 3 the method of order 2*s* has the matrix of coefficients

$$A = \begin{bmatrix} \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} \\ \frac{5}{36} + \frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} \\ \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} \end{bmatrix}$$

And there is a matrix *S* such that

$$S^{-1}AS=\bar{A}=\begin{bmatrix} a_1 & a_1-b_1 & 0 \\ a_1+b_1 & a_1 & 0 \\ 0 & 0 & a_2 \end{bmatrix}=A_1\oplus A_2,$$

where $a_1\simeq 0.142342788,\ b_1\simeq 0.196731007,\ a_2\simeq 0.215314423$

And a numerical calculation gives

$$S\simeq\begin{bmatrix} -0.0455241821 & 0.0441943589 & 0.0721518521 \\ -0.140048242 & -0.139620426 & 0.118832579 \\ 1.0 & -0.244595668 & 1.0 \end{bmatrix}$$

Where the columns are eigenvectors of $[a_1I-A]^2$.

Let $D=D_1\oplus D_2$ and $L=L_1\oplus L_2$ so that the result of the **Theorem 1** may be applied using (14), we get

$$\rho[M_1(z)]\le 1-\left(\frac{a_1}{b_1}\right)^2 \simeq 0.4765 \text{ For all } z \in C^-.$$

On the other hand, since $D_2=[l_{33}]$ and $L_2=[0]$, gives

$$M_2(z)=0 \quad \text{implies} \quad \rho[M_2(z)]=0.$$

Then

$$\rho\left[\bar{M}(z)\right]= 0.4765 \text{ for all } z\in\mathbb{C}^-$$

and in this case we obtain

$$Q^HQ=\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{b_1-a_1}{b_1+a_1} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \qquad (15)$$

Next, consider the four-stage Gauss method with matrix of coefficients $A=\left[a_{ij}\right]$ obtained by solving the sets of equations

$$\sum_{j=1}^{4} a_{ij}c_j^{r-1}=\frac{c_i^r}{r}, \quad r=1,2,3,4, \text{ for each } i=1,2,3,4,$$

where c_1,c_2,c_3,c_4 are the zeros of $P_4(2x-1)$, the transformed legendre polynomial of degree 4. The elements of the transformed matrix

$$S^{-1}AS=\bar{A}=\begin{bmatrix} a_1 & a_1+b_1 & 0 & 0 \\ a_1+b_1 & a_1 & 0 & 0 \\ 0 & 0 & a_2 & a_2+b_2 \\ 0 & 0 & a_2+b_2 & a_2 \end{bmatrix}=A_1\oplus A_2,$$

where $a_1\simeq 0.091566240,\ a_2\simeq 0.158433760,\ b_1\simeq 0.147520224,$ $b_2\simeq 0.165384116$ and

$$S\simeq\begin{bmatrix} 0.063771667 & -0.054434907 & -0.231157907 & 0.013395896 \\ -0.027613999 & 0.161524607 & -0.083606572 & -0.040682019 \\ -0.784055901 & -0.290017081 & -0.859410259 & -0.266775537 \\ 1.0 & -1.164674610 & 1.0 & -1.364336800 \end{bmatrix}$$

Where the columns are eigenvectors of $[a_1I-A]^2$ and $[a_2I-A]^2$. Again the result of the **Theorem 1** may be applied using (14), we obtain

$$\rho[M_1(z)]\le 1-\left(\frac{a_1}{b_1}\right)^2 \simeq 0.6147, \text{ for all } z\in\mathbb{C}^-$$

$$\rho[M_2(z)]\le 1-\left(\frac{a_1}{b_1}\right)^2 \simeq 0.0823, \text{ for all } z\in\mathbb{C}^-$$

Where the matrices *D* and *L* are given by

$$L=L_1\oplus L_2=\begin{bmatrix} 0 & 0 & 0 & 0 \\ l_{21} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & l_{43} & 0 \end{bmatrix},\ D=D_1\oplus D_2=\begin{bmatrix} l_{11} & 0 & 0 & 0 \\ 0 & l_{22} & 0 & 0 \\ 0 & 0 & l_{33} & 0 \\ 0 & 0 & 0 & l_{44} \end{bmatrix}.$$

Then

$$\rho\left[\bar{M}(z)\right]=0.6147 \text{ for all } z\in\mathbb{C}^-$$

and we obtain

$$Q^HQ=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{b_1-a_1}{b_1+a_1} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \frac{b_2-a_2}{b_2+a_2} \end{pmatrix}. \qquad (16)$$

4. NUMERICAL RESULTS

In this section, a number of numerical experiments were carried out in order to evaluate the efficiency of the proposed class of general non-linear scheme. Results for three non-linear initial value problems are reported and compared with results obtained using the scheme described in Cooper and Butcher [1].

Problem 1 denotes the non-linear system

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

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

Problem 2 is also the non-linear system

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

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

Problem 3 Insulator physics non-linear problem

$$x_1' = -x_1 + 10^8 x_3 (1 - x_1), \qquad x_1(0) = 1,$$
$$x_2' = -10x_2 + 3\times 10^7 x_3 (1 - x_2), \qquad x_2(0) = 0,$$
$$x_3' = -x_1' - x_2', \qquad x_3(0) = 0,$$

Where the eigenvalues of the Jacobian at the initial point are 0, -1.0 and -3.0$\times 10^7$.

For each problem, a single step was carried out, in each method, using the Jacobian evaluated at the initial point. For each scheme tested, the initial iterate Y^0 is chosen as $Y^0 = e \otimes x,$ where *x* is the true solution at the initial point.

Method 1 denotes the three-stage Gauss method implemented according to the basic scheme (5) with parameters given in Cooper and Butcher [1] with relaxation parameter $\omega = 1.$

Method 1^* denotes the three-stage Gauss method but implemented using the non-linear scheme (9) proposed here with the matrix *Q* given by (15) and E^m chosen from the scheme (5).

Method 2 denotes the four-stage Gauss method implemented according to the basic scheme (5) with parameters given in Cooper and Butcher [1] with relaxation parameter $\omega = 1.$

Table 1. Values of *m* giving $e_m \leq 10^{-9}$ for Gauss method

Problems	Step size	Methods			
		1	1^*	1	2^*
1	h = 10^{-5}	6	3	3	2
2	h = 2×10^{-6}	7	3	8	2
3	h = 3.3×10^{-8}	8	3	10	2

Method 2^* denotes the four-stage Gauss method but implemented using the non-linear scheme (9) proposed here with the matrix Q given by (16) and E^m chosen from the scheme (5).
For each problem the quantities

$$e_m = \left\| Y^m - Y^{m-1} \right\|_\infty, \quad m = 1, 2, 3, \ldots,$$

Are calculated. The values of $e_m \leq \mathrm{TOL} = 10^{-9}$ are tabulated for each problem and method. Similar results are obtained for different values of TOL. The Results are given in table 1.

5. Conclusion

Numerical result shows that, the proposed class of general non-linear iteration scheme accelerates the convergence rate of the general linear iteration scheme proposed by Cooper and Butcher [1] for some stiff problems that has strong stiffness. It will be possible to apply the proposed class of general non-linear scheme to accelerate the rate of convergence of other linear iteration schemes.

Conflict of Interests

The authors declare that there is no conflict of interest related to the publication of this article.

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