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SEQUENTIAL SECOND DERIVATIVE GENERAL LINEAR METHODS FOR STIFF SYSTEMS

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ABSTRACT. Second derivative general linear methods (SGLMs) as an extension of general linear methods (GLMs) have been introduced to improve the stability and accuracy properties of GLMs. The coefficients of SGLMs are given by six matrices, instead of four matrices for GLMs, which are obtained by solving nonlinear systems of order and usually Runge–Kutta stability conditions. In this paper, we introduce a technique for construction of an special case of SGLMs which decreases the complexity of finding coefficients matrices.

Keywords: General linear methods, two-derivative methods, ordinary differential equation, order conditions, A- and L-stability.
MSC(2010): Primary: 65L05.

1. **Introduction**

Numerous methods have been introduced to approximate the solution of an autonomous ordinary differential equation in the form

$$\begin{aligned} &y'(x) = f(y(x)), \qquad x \in [x_0, \overline{x}], \\ &y(x_0) = y_0, \end{aligned} \tag{1.1}$$

where $f : \mathbb{R}^m \to \mathbb{R}^m$ and m is the dimensionality of the system. In designing of algorithms, there is always a conflict between the following three basic aims:

- good accuracy using high order methods,

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- good stability properties, especially A-stability, in the case of solving stiff problems,
- modest computational costs.

Construction of the methods, considering these aims, puts severe restrictions. Since it has been shown that the order of A-stable implicit linear multistep method cannot exceed two (second Dahlquist barrier [22]), also Iserles and Nørsett [31] have shown that the order of a Runge–Kutta method cannot exceed $s + 1$ where s is the number of the sequential stages. Hence, search for new techniques different than traditional ones is a great challenge.

Many codes have been introduced for solving (1.1) in the class of linear multistep methods with good accuracy and reasonably wide region of absolute stability which use first derivatives of the solution (for instance [19, 21, 24, 27, 28, 29]) and many other methods which use first and second derivatives of the solution [20, 23, 30]. By adding a linear multistep flavor to the Runge–Kutta methods, some methods have been introduced such as the pseudo Runge–Kutta methods of Byrne and Lambert [18], and the multistep Runge–Kutta methods of Burrage [17]. Also some of the introduced methods add Runge–Kutta flavor to linear multistep methods, such as the hybrid, generalized multistep and modified multistep methods developed by Gear [25], Gragg and Stetter [26], and Butcher [5].

General linear methods (GLMs) were introduced in 1966 by Butcher [6] as a unified approach for the study of consistency, stability and convergence of the Runge–Kutta and linear multistep methods. This discovery opened the possibility of obtaining essentially new methods which were neither Runge–Kutta nor linear multistep methods and nor slight variations of these methods. Burrage and Butcher used a partitioned $(s+r)\times(s+r)$ matrix to represent a GLM which contains four matrices A, U, B and V, and has the form

$$\left[\begin{array}{c|c} A_{s\times s} & U_{s\times r} \\ \hline B_{r\times s} & V_{r\times r} \end{array}\right],$$

where r is the number of input and output approximations, and s is the number of internal stages. The coefficients of these matrices indicate the relationships among various numerical quantities that arise in the computation. As for the Runge–Kutta methods, the structure of the leading coefficients matrix A determines the implementation costs of these methods. As members of GLMs, to achieve good damping of the error with modest computational cost, diagonally implicit multistage integration methods (DIMSIMs) were introduced by Butcher in [7, 9] and were extended by Butcher and Jackiewicz in [13, 14, 15, 16, 32]. These methods are considerably potential for efficient implementation due to the availability of parallelism (structure of the leading matrix A) and lower the cost of implementation. In 1995, Butcher and Chartier [11] proposed that it is more desirable to construct parallel GLMs with L-stability property with $M(\infty)=0$, where $M(z)=V+zB(I-zA)^{-1}U$ is the stability matrix of the method. This ensures that, in the situation of differential algebraic equations, the numerical solution lies on the constraint manifold.

On the other hand, GLMs were extended in which second derivatives of the solution, as well as first derivatives, can be calculated. These methods were introduced by Butcher and Hojjati in [12] and studied more by Abdi and Hojjati [3, 4]. A second derivative general linear method (SGLM) is characterized by (p,q,r,s) and six matrices denoted by $A,\overline{A}\in\mathbb{R}^{s\times s}$, $U\in\mathbb{R}^{s\times r}$, $B,\overline{B}\in\mathbb{R}^{r\times s}$, and $V\in\mathbb{R}^{r\times r}$, where p and q are respectively order and stage order of the method, r is the number of input and output approximations, and s is the number of internal stages. Let $Y^{[n]}=[Y_i^{[n]}]_{i=1}^s$ be an approximation of stage order q to the vector $y(x_{n-1}+ch)=[y(x_{n-1}+c_ih)]_{i=1}^s$, where $c=[c_1\ c_2\ \cdots\ c_s]^T$ is the abscissa vector, and the vectors $f(Y^{[n]})=[f(Y_i^{[n]})]_{i=1}^s$ and $g(Y^{[n]})=[g(Y_i^{n})]_{i=1}^s$ denote the stage first and second derivative values, where $g(\cdot)=f'(\cdot)f(\cdot)$. Also denote by $y^{[n-1]}=[y_i^{[n-1]}]_{i=1}^r$ and $y^{[n]}=[y_i^{[n]}]_{i=1}^r$, the input and output vectors at step number n respectively. An SGLM used for the numerical approximation of the solution of (1.1) is given by

$$\begin{aligned} Y^{[n]} &= h(A\otimes I_m)f(Y^{[n]})+h^2(\overline{A}\otimes I_m)g(Y^{[n]})+(U\otimes I_m)y^{[n-1]},\\ y^{[n]} &= h(B\otimes I_m)f(Y^{[n]})+h^2(\overline{B}\otimes I_m)g(Y^{[n]})+(V\otimes I_m)y^{[n-1]}, \end{aligned} \tag{1.2}$$

where $n=1,2,\cdots,N$, $Nh=\overline{x}-x_0$, h is the stepsize and $\otimes$ is the Kronecker product of two matrices. It is convenient to write coefficients of the method, that is, elements of A, $\overline{A}$, U, B, $\overline{B}$ and V, as a partitioned $(s+r)\times(2s+r)$ matrix

$$\left[\begin{array}{c|c|c} A & \overline{A} & U \\ \hline B & \overline{B} & V \end{array}\right].$$

Construction and basic concepts of SGLMs have been studied in [3, 4, 12]. Because of lower cost computing, it is always assumed that the matrices $A=[a_{ij}]$ and $\overline{A}=[\overline{a}_{ij}]$ have the lower triangular form with

$\lambda = a_{11} = a_{22} = \cdots = a_{ss}$ and $\mu = \overline{a}_{11} = \overline{a}_{22} = \cdots = \overline{a}_{ss}$. In [3] the authors have divided SGLMs into four types, depending on the nature of the differential system to be solved and the computer architecture that is used to implement these methods. Types 1 and 2 are those with arbitrary a_{ij}, $\overline{a}_{ij}$ where $\lambda = \mu = 0$ and $\lambda > 0, \mu < 0$, respectively. Such methods are appropriate respectively for nonstiff and stiff differential systems in a sequential computing environment. Requiring $a_{ij} = \overline{a}_{ij} = 0$, cases $\lambda = \mu = 0$ and $\lambda > 0$, $\mu < 0$ lead respectively to types 3 and 4 methods which can be useful respectively for non-stiff and stiff systems in a parallel computing environment.

Second derivative diagonally implicit multistage integration methods (SDIMSIMs) as a subclass of SGLMs have been introduced in [3] in four types, together with their intended applications (for nonstiff or stiff ODEs) and architectures (sequential or parallel). Order barriers for parallel SDIMSIMs, type two and generalized type four SGLMs with Runge–Kutta stability (RKS) property have been discussed in [3, 4]. The obtained order barriers have been confirmed via order arrows by Abdi and Butcher [1], too. To study more about order arrows, references are made to [2, 8, 10] which include applications and a discussion of order arrows.

In this paper, we introduce a new formula which causes the order conditions and the stability matrix of SGLMs take simpler form. The constructed A-stable methods are L-stable too.

Next sections of this paper are organized as follows: in Section 2, we introduce an special case of SGLMs as A-$\overline{A}$-V methods. Construction of A-$\overline{A}$-V methods with RKS property of order $p = q \leq 4$ is given in Section 3, and the paper is closed in Section 4, by giving some numerical experiments to confirm efficiency of the constructed methods.

2. A-$\overline{\mathbf{A}}$-V methods

In this section, we first recall the order conditions of SGLMs that have been discussed in [4]. The method (1.2) has order p and stage order q if

$$y^{[n-1]} = \sum_{k=0}^{p} h^k \left(\alpha_k \otimes y^{(k)}(x_{n-1})\right) + O(h^{p+1}) \tag{2.1}$$

implies that

$$Y^{[n]} = \sum_{k=0}^{p} h^k \left(\frac{c^k}{k!} \otimes y^{(k)}(x_{n-1}) \right) + O(h^{q+1}) \tag{2.2}$$

and

$$y^{[n]} = \sum_{k=0}^{p} h^k \left(\alpha_k \otimes y^{(k)}(x_n) \right) + O(h^{p+1}), \tag{2.3}$$

for some vectors $\alpha_0, \alpha_1, \dots, \alpha_p \in \mathbb{R}^r$ associated with the method. Here, c^k denotes component-wise powers of abscissae vector c. The conditions for (1.2) to have order p and stage order q have been obtained by Abdi and Hojjati in [4]. Let us denote $Z := [1 \;\; z \;\; \cdots \;\; z^p]^T \in \mathbb{C}^{p+1}$ and collect the vectors α_k in the matrix W defined by

$$W = \left[\begin{array}{cccc} \alpha_0 & \alpha_1 & \cdots & \alpha_p \end{array} \right]. \tag{2.4}$$

Theorem 2.1. [4] *Assume that $y^{[n-1]}$ satisfies (2.1). Then the SGLM (1.2) of order p and stage order $q = p$ satisfies (2.2) and (2.3) if and only if*

$$e^{cz} = zAe^{cz} + z^2\overline{A}e^{cz} + UWZ + O(z^{p+1}), \tag{2.5}$$

$$e^{z}WZ = zBe^{cz} + z^2\overline{B}e^{cz} + VWZ + O(z^{p+1}), \tag{2.6}$$

where e^{cz} denotes the vector with components given by $e^{c_i z}$, $i = 1, 2, \dots, s$.

If $U = I_s$, the matrix W is given by

$$W = C - ACK - \overline{A}CK^2, \tag{2.7}$$

where $C = (C_{ij}) \in \mathbb{R}^{s\times(p+1)}$ is the Vandermonde matrix with coefficients

$$C_{ij} = \frac{c_i^{j-1}}{(j-1)!}, \quad 1 \le i \le s, \quad 1 \le j \le p+1,$$

and $K \in \mathbb{R}^{(p+1)\times(p+1)}$ is the shifting matrix defined by $K = [0 \;\; e_1 \;\; \cdots \;\; e_p]$ with e_j as the jth unit vector (see [4]).

In general, it is a very complicated task to construct an SGLM that possess RKS, especially for the methods with a large number of r and s, since this requires the solution of large systems of polynomial equations of high degree for the unknown coefficients of the methods. However, it is possible to simplify the analysis and construction of the methods by some restrictions on the coefficients matrices.

Here, we are looking for SGLMs with $B = VA$. For an SGLM, the stability matrix obtained by a standard linear stability analysis takes the form $M(z) = V + \left(zB + z^2\overline{B}\right)\left(I - zA - z^2\overline{A}\right)^{-1}U$. While the condition $\rho(M(\infty)) = 0$, which guaranties L-stability property, is sufficient to achieve a good damping of the errors, it may seem even more desirable to require $M(\infty) = 0$. To achieve this aim, we choose $U = I_s$ and $\overline{B} = V\overline{A}$. These restrictions also reduce the number of unknown coefficients and simplify the analysis and construction of the methods. Considering these relations, order conditions of the methods take a particular form:

Theorem 2.2. *Let $p = r - 1 = s - 1$ and denote by $l_j(x)$, the jth lagrange polynomial based on the abscissae c_j, $j = 1, \ldots, s$. Then an SGLM of the form*

$$\left[\begin{array}{c|c|c} A & \overline{A} & I \\ \hline VA & V\overline{A} & V \end{array}\right] \tag{2.8}$$

has order p and stage order $q = p$ if and only if

$$V = L - AL' - \overline{A}L'', \tag{2.9}$$

where the (i,j) elements of L, L' and L'' are respectively given by $l_j(1+c_i), l_j'(1+c_i)$ and $l_j''(1+c_i)$.

Proof. Since $p = q = r - 1$, from (2.5), the vector valued function WZ takes the form $WZ = (I - zA - z^2\bar{A})e^{cz} + O(z^r)$. Substituting WZ into (2.6), the order conditions can be written as

$$Ve^{cz} = (I - zA - z^2\overline{A})e^{(\mathrm{e}+c)z} + O(z^r),$$

where $\mathrm{e} = [1, 1, \ldots, 1]^T \in \mathbb{R}^s$, $e^{cz} = [e^{c_1 z}, \ldots, e^{c_s z}]^T$ and $e^{(\mathrm{e}+c)z} = [e^{(1+c_1)z}, \ldots, e^{(1+c_s)z}]^T$. This implies that

$$VP(c) = P(\mathrm{e} + c) - AP'(\mathrm{e} + c) - \overline{A}P''(\mathrm{e} + c),$$

for all polynomials of degree less than $r - 1$. Taking $P(x) = l_j(x)$ for $j = 1, \ldots, s$, then gives the coefficients of V as (2.9). □

Now, we show the non-existence of parallel A-$\overline{A}$-V SGLMs of types 3 and 4 with RKS property.

Theorem 2.3. *Parallel SGLMs of the form* (2.8) *with RKS property do not exist for nonstiff and stiff systems.*

Proof. The stability matrix for parallel SGLMs of the form (2.8) is given by

$$M(z) = \frac{1}{1 - \lambda z - \mu z^2} V,$$

hence

$$\mathrm{tr}(M(z)) = \mathrm{tr}(V) \times \left(1 + \lambda z + (\mu + \lambda^2) z^2 + (2\lambda\mu + \lambda^3) z^3 + O(z^4)\right).$$

Since RKS is required, we must have $\mathrm{tr}(M(z)) = e^z + O(z^{p+1})$. So, if $\lambda = \mu = 0$ (methods for nonstiff systems), we can not take any order, i.e. there is no any parallel SGLMs of the form (2.8) for nonstiff systems. In the case of parallel methods for stiff systems, the maximum obtainable order is 2 when $\lambda = 1$, $\mu = -\frac{1}{2}$ and $\mathrm{tr}(V) = 1$. But the last condition is impossible because by these values for λ and μ, we have

$$\mathrm{tr}(V) = \mathrm{tr}(L - \lambda\, L' - \mu\, L'') = s = p + 1 > 1.$$

□

The stability matrix of A-$\overline{A}$-V methods is

$$M(z) = V\left(I + \left(zA + z^2\overline{A}\right)\left(I - zA - z^2\overline{A}\right)^{-1}\right).$$

RKS property causes that the $r-1$ number eigenvalues of V be zero. Also, noting that $\sum_{j=1}^{s} l_j(x) = 1$, it is easy to conclude $V\mathrm{e} = \mathrm{e}$, $\mathrm{e} = [1, 1, \ldots, 1]^T \in \mathbb{R}^s$, which means the only nonzero eigenvalue of V is 1. So the A-$\overline{A}$-V methods with RKS property are zero-stable.

3. Construction of A-$\overline{\text{A}}$-V methods with RKS

In this section, we construct A-$\overline{A}$-V methods of type 2 with RKS property up to order $p = 4$ with $p = q = r - 1 = s - 1$. All the constructed methods are L-stable. We will consider throughout the paper, the vector c of abscissae to be values uniformly in the interval $[0, 1]$ so that

$$c = \begin{bmatrix} 0 & \dfrac{1}{s-1} & \cdots & \dfrac{s-2}{s-1} & 1 \end{bmatrix}^T.$$

3.1. **Methods of order** $p = 1$**.** The coefficients matrices of these methods take the form

$$A = \begin{bmatrix} \lambda & 0 \\ a_{21} & \lambda \end{bmatrix}, \overline{A} = \begin{bmatrix} \mu & 0 \\ \overline{a}_{21} & \mu \end{bmatrix}, V = \begin{bmatrix} \lambda & 1-\lambda \\ -1 + a_{21} + \lambda & 2 - a_{21} - \lambda \end{bmatrix},$$

$$B = VA, \qquad \overline{B} = V\overline{A}, \qquad U = I.$$

Since here $p = r - 1 = 1$, so RKS property is achieved when $\det(M(z)) = 0$, and this leads to $a_{21} = 1$. We are looking for the values of λ and

μ which guarantee A-stability property. To do this, we consider the stability function of the methods in the form

$$R(z) = \frac{1 + n_1 z + n_2 z^2}{(1 - \lambda z - \mu z^2)^2},$$

where the order conditions imply that

$$1 + n_1 z + n_2 z^2 = \exp(z)(1 - \lambda z - \mu z^2)^2 - C_1 z^2 + O(z^3),$$

where C_1 is constant. Using E-polynomial theorem, A-stability is achieved iff $\lambda > 0$, $\mu < 0$, and $E(y)$ is non-negative for all real y where the E-polynomial is defined by

$$E(y) = |1 - \lambda \mathbf{i} y + \mu y^2|^4 - |1 + n_1 \mathbf{i} y - n_2 y^2|^2,$$

where $\mathbf{i}$ is the imaginary unit. By choosing $C_1 = \frac{1}{1000}$, a detailed calculation shows that

$$E(y) = y^4\big(E_0 + E_1 y^2 + E_2 y^4\big),$$

where

$$\begin{aligned}
E_0 &= 8\mu\lambda^2 + 2\mu^2 + \frac{499}{250}\mu - \frac{2499}{500}\lambda^2 + 4\lambda^3 + \frac{499}{250}\lambda - 8\lambda\mu - \frac{249001}{1000000},\\
E_1 &= 2\lambda^2\mu^2 + 4\mu^3,\\
E_2 &= \mu^4.
\end{aligned}$$

We need to choose λ and μ such that $E_0 + E_1 x + E_2 x^2$ is never negative for all positive real numbers x, and so that $\lambda > 0$, $\mu < 0$. Pairs of (λ, μ) values in domain $[0, 2] \times [-1, 0]$ giving A-stability are shown in Figure 1(A). We select a single example, characterized by $\lambda = \frac{4}{5}$, $\mu = -\frac{3}{10}$. In the constructed methods, $\overline{a}_{21}$ is as a free parameter which by choosing $\overline{a}_{21} = 0$, the coefficients of the method take the form

$$\left[\begin{array}{cc|cc|cc}
\frac{4}{5} & 0 & -\frac{3}{10} & 0 & 1 & 0\\
1 & \frac{4}{5} & 0 & -\frac{3}{10} & 0 & 1\\
\hline
\frac{21}{25} & \frac{4}{25} & -\frac{6}{25} & -\frac{3}{50} & \frac{4}{5} & \frac{1}{5}\\
\frac{21}{25} & \frac{4}{25} & -\frac{6}{25} & -\frac{3}{50} & \frac{4}{5} & \frac{1}{5}
\end{array}\right].$$

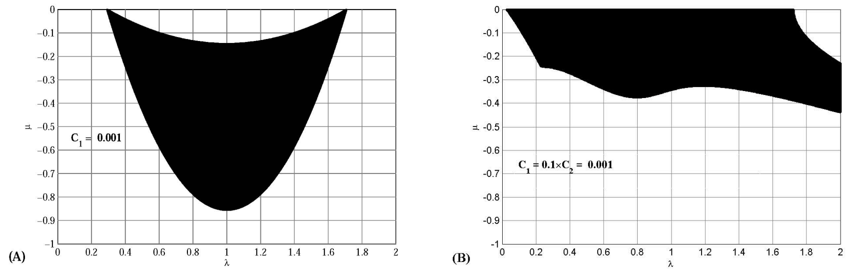

Figure 1. A-stable choices of (λ, μ): (A) in domain $[0, 2] \times [-1, 0]$ for $p = s - 1 = 1$, (B) in domain $[0, 2] \times [-1, 0]$ for $p = s - 1 = 2$.

We note that this L-stable method is not a genuine SGLM with $r = 2$, because it reduces to the SGLM with $r = 1$ (TDRK) given by

$$\begin{array}{c|c|c} c & A & \overline{A} \\ \hline & b^T & \overline{b}^T \end{array} = \begin{array}{c|cc|cc} 0 & \frac{4}{5} & 0 & -\frac{3}{10} & 0 \\ 1 & 1 & \frac{4}{5} & 0 & -\frac{3}{10} \\ \hline & \frac{21}{25} & \frac{4}{25} & -\frac{6}{25} & -\frac{3}{50} \end{array}$$

3.2. **Methods of order $p = 2$.** In this subsection, we describe how to construct methods with $p = 2$. These methods take the form

$$A = \begin{bmatrix} \lambda & 0 & 0 \\ a_{21} & \lambda & 0 \\ a_{31} & a_{32} & \lambda \end{bmatrix}, \quad \overline{A} = \begin{bmatrix} \mu & 0 & 0 \\ \overline{a}_{21} & \mu & 0 \\ \overline{a}_{31} & \overline{a}_{32} & \mu \end{bmatrix}, \quad V = L - AL' - \overline{A}L'',$$

$$B = VA, \qquad \overline{B} = V\overline{A}, \qquad U = I.$$

As the previous subsection, firstly we need to find the values of λ and μ for A-stability. The stability function has the form

$$R(z) = \frac{1 + \sum_{j=1}^{4} n_j z^j}{(1 - \lambda z - \mu z^2)^3},$$

where, considering the order conditions, we have

$$1 + \sum_{j=1}^{4} n_j z^j = \exp(z)(1 - \lambda z - \mu z^2)^3 - \sum_{j=1}^{2} C_j z^{j+2} + O(z^5),$$

where C_1 and C_2 are constants. For these methods the E-polynomial is defined by

$$E(y) = |1 - \lambda \mathbf{i} y + \mu y^2|^6 - \left| 1 + \sum_{j=1}^{4} n_j (\mathbf{i} y)^j \right|^2,$$

which leads to

$$E(y) = y^4 \big(E_0 + E_1 y^2 + E_2 y^4 + E_3 y^6 + E_4 y^8 \big),$$

where the coefficients are expressions in λ, μ and C_j for $j = 1, 2$. By choosing $C_1 = 0.1 \times C_2 = \frac{1}{1000}$, we need to choose λ and μ such that $E_0 + E_1 x + E_2 x^2 + E_3 x^3 + E_4 x^4$ is never negative for all positive real numbers x, and so that $\lambda > 0$, $\mu < 0$. Pairs of (λ, μ) values in domain $[0, 2] \times [-1, 0]$ giving A-stability are shown in Figure 1 (B). We present here just a single example, characterized by $\lambda = \frac{3}{4}$, $\mu = -\frac{1}{4}$. RKS conditions imply that

$$a_{21} = \frac{1}{2}, \quad a_{31} = 1 - a_{32}, \quad \overline{a}_{21} = -\frac{1}{4}, \quad \overline{a}_{31} = -\frac{1}{4} - \frac{1}{2} a_{32} - \overline{a}_{32},$$

with free parameters a_{32} and $\overline{a}_{32}$. By choosing $a_{32} = \overline{a}_{32} = 0$, the coefficients of the method take the form

$$\left[\begin{array}{ccc|ccc|ccc}
\frac{3}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 & 1 & 0 & 0 \\
\frac{1}{2} & \frac{3}{4} & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 & 1 & 0 \\
1 & 0 & \frac{3}{4} & -\frac{1}{4} & 0 & -\frac{1}{4} & 0 & 0 & 1 \\
\hline
\frac{7}{16} & \frac{3}{4} & -\frac{3}{16} & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{16} & \frac{1}{4} & 1 & -\frac{1}{4} \\
\frac{7}{16} & \frac{3}{4} & -\frac{3}{16} & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{16} & \frac{1}{4} & 1 & -\frac{1}{4} \\
\frac{7}{16} & \frac{3}{4} & -\frac{3}{16} & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{16} & \frac{1}{4} & 1 & -\frac{1}{4}
\end{array}\right].$$

Again this L-stable method is not a genuine SGLM with $r = 3$, because it reduces to the SGLM with $r = 1$ (TDRK) given by

$$\begin{array}{c|c|c}
c & A & \overline{A} \\
\hline
 & b^T & \overline{b}^T
\end{array}
=
\begin{array}{c|ccc|ccc}
0 & \frac{3}{4} & 0 & 0 & -\frac{1}{4} & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & \frac{3}{4} & 0 & -\frac{1}{4} & -\frac{1}{4} & 0 \\
1 & 1 & 0 & \frac{3}{4} & -\frac{1}{4} & 0 & -\frac{1}{4} \\
\hline
 & \frac{7}{16} & \frac{3}{4} & -\frac{3}{16} & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{16}
\end{array}$$

3.3. **Methods of order $p = 3$.** In this subsection, we describe how to construct methods with $p = 3$. These methods take the form

$$A = \begin{bmatrix} \lambda & 0 & 0 & 0 \\ a_{21} & \lambda & 0 & 0 \\ a_{31} & a_{32} & \lambda & 0 \\ a_{41} & a_{42} & a_{43} & \lambda \end{bmatrix}, \quad \overline{A} = \begin{bmatrix} \mu & 0 & 0 & 0 \\ \overline{a}_{21} & \mu & 0 & 0 \\ \overline{a}_{31} & \overline{a}_{32} & \mu & 0 \\ \overline{a}_{41} & \overline{a}_{42} & \overline{a}_{43} & \mu \end{bmatrix},$$

$$V = L - AL' - \overline{A}L'', \qquad B = VA, \quad \overline{B} = V\overline{A}, \qquad U = I.$$

Following the previous subsections, we first find λ and μ for A-stability. The stability function has the form

$$R(z) = \frac{1 + \sum_{j=1}^{6} n_j z^j}{(1 - \lambda z - \mu z^2)^4},$$

where, because of the order conditions,

$$1 + \sum_{j=1}^{6} n_j z^j = \exp(z)(1 - \lambda z - \mu z^2)^4 - \sum_{j=1}^{3} C_j z^{j+3} + O(z^7),$$

where C_j for $j = 1, 2, 3$ are constants. For these methods the E-polynomial is given by

$$E(y) = |1 - \lambda \mathbf{i} y + \mu y^2|^8 - \left| 1 + \sum_{j=1}^{6} n_j (\mathbf{i} y)^j \right|^2 = y^4 \sum_{j=0}^{6} E_j \, y^{2j},$$

where the coefficients E_j, $j = 1, 2, \cdots, 6$, are expressions in λ, μ and C_j for $j = 1, 2, 3$. By choosing $C_1 = -0.1 \times C_2 = 0.1 \times C_3 = \frac{1}{1000}$, we need to choose λ and μ such that $E_0 + E_1 x + E_2 x^2 + E_3 x^3 + E_4 x^4 + E_5 x^5 + E_6 x^6$ is never negative for all positive real numbers x, and so that $\lambda > 0$, $\mu < 0$. Pairs of (λ, μ) values in domain $[0, 2] \times [-1, 0]$ giving A-stability are shown in Figure 2(A). Here, we present a single example characterized by $\lambda = \frac{9}{10}$, $\mu = -\frac{1}{6}$. To decrease the complexity of the nonlinear system of RKS conditions, we set the free parameters as $a_{21} = \overline{a}_{21} = \overline{a}_{31} = 0$. In order to find the coefficient matrices, for orders greater than or equal to 3, it is not possible to solve nonlinear equations (RKS conditions) symbolically. So, this system of nonlinear equations is solved numerically using the fsolve.ms command from Maple. The coefficients matrices of

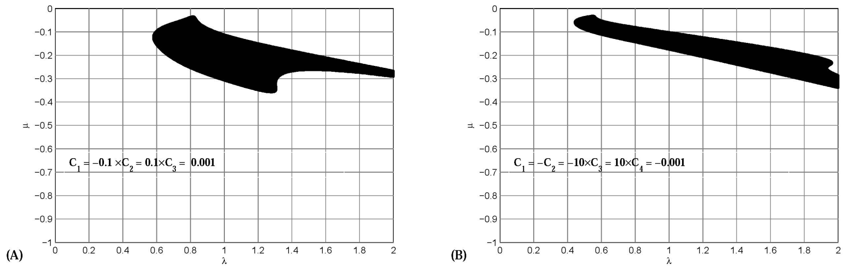

FIGURE 2. A-stable choices of (λ, μ): (A) in domain $[0,2] \times [-1,0]$ for $p = s-1 = 3$, (B) in domain $[0,2] \times [-1,0]$ for $p = s-1 = 4$.

the method are given by

$$A = \begin{bmatrix} 0.9000000000 & 0 & 0 & 0 \\ 0 & 0.9000000000 & 0 & 0 \\ 0.4265391445 & -0.4633831628 & 0.9000000000 & 0 \\ 1.0494647217 & -1.1903827725 & 0.0768604217 & 0.9000000000 \end{bmatrix},$$

$$\overline{A} = \begin{bmatrix} -0.1666666667 & 0 & 0 & 0 \\ 0 & -0.1666666667 & 0 & 0 \\ 0 & -0.3324263751 & -0.1666666667 & 0 \\ -0.0108264219 & -0.7653253688 & -0.0429696149 & -0.1666666667 \end{bmatrix},$$

$$V = \begin{bmatrix} -0.6000000000 & 1.9500000000 & 0.6000000000 & -0.9500000000 \\ 0.9500000000 & -4.4000000000 & 7.6500000000 & -3.2000000000 \\ -4.9057430034 & 16.90448190256 & -18.5022668497 & 7.5035279506 \\ -14.3819290817 & 51.7739521261 & -60.8942898941 & 24.5022668497 \end{bmatrix}.$$

3.4. **Methods of order $p = 4$.** In this subsection, we construct methods with $p = 4$ which take the form

$$A = \begin{bmatrix} \lambda & 0 & 0 & 0 & 0 \\ a_{21} & \lambda & 0 & 0 & 0 \\ a_{31} & a_{32} & \lambda & 0 & 0 \\ a_{41} & a_{42} & a_{43} & \lambda & 0 \\ a_{51} & a_{52} & a_{53} & a_{54} & \lambda \end{bmatrix}, \quad \overline{A} = \begin{bmatrix} \mu & 0 & 0 & 0 & 0 \\ \overline{a}_{21} & \mu & 0 & 0 & 0 \\ \overline{a}_{31} & \overline{a}_{32} & \mu & 0 & 0 \\ \overline{a}_{41} & \overline{a}_{42} & \overline{a}_{43} & \mu & 0 \\ \overline{a}_{51} & \overline{a}_{52} & \overline{a}_{53} & \overline{a}_{54} & \mu \end{bmatrix},$$

$$V = L - AL' - \overline{A}L'', \qquad B = VA, \quad \overline{B} = V\overline{A}, \quad U = I.$$

At first, we consider how to choose λ and μ to ensure the A-stability property. We look for methods for which the stability function has the form

$$R(z)=\frac{1+\sum_{j=1}^{8}n_j z^j}{(1-\lambda z-\mu z^2)^5},$$

where, because of the order conditions,

$$1+\sum_{j=1}^{8}n_j z^j=\exp(z)(1-\lambda z-\mu z^2)^5-\sum_{j=1}^{4}C_j z^{j+4}+O(z^9),$$

where C_j for $j=1,2,3,4$ are constants. E-polynomial of these methods is given by

$$E(y)=|1-\lambda\mathbf{i}y+\mu y^2|^{10}-\left|1+\sum_{j=1}^{8}n_j(\mathbf{i}y)^j\right|^2=y^6\sum_{j=0}^{7}E_j y^{2j},$$

where the coefficients E_j are expressions in λ, μ and C_j for $j=1,2,3,4$. By choosing $C_1=-C_2=-10\times C_3=10\times C_4=-\frac{1}{1000}$, the pairs of (λ,μ) values in domain $[0,2]\times[-1,0]$ giving A-stability are shown in Figure 2(B). We select single example, characterized by $\lambda=\frac{3}{5}$, $\mu=-\frac{1}{10}$. Setting the free parameters as $a_{21}=a_{31}=\overline{a}_{21}=\overline{a}_{31}=0$ in order to make calculation easier, RKS conditions and equation (2.9) make the coefficients matrices of the method to take the following forms

$$A=\begin{bmatrix} 0.6000000000 & 0 & 0 & 0 & 0\\ 0 & 0.6000000000 & 0 & 0 & 0\\ 0 & 0.8457481365 & 0.6000000000 & 0 & 0\\ 0.0272278796 & 1.5134875394 & 0.2025300085 & 0.6000000000 & 0\\ 0.1074165413 & 1.6644692218 & 0.6792600911 & -0.0701360165 & 0.6000000000 \end{bmatrix},$$

$$\overline{A}=\begin{bmatrix} -0.1000000000 & 0 & 0 & 0 & 0\\ 0 & -0.1000000000 & 0 & 0 & 0\\ 0 & -0.2391700148 & -0.1000000000 & 0 & 0\\ -0.0082050510 & -0.4277671880 & -0.0720469981 & -0.1000000000 & 0\\ -0.0081636294 & -0.5604020695 & -0.0624274119 & -0.0455594803 & -0.1000000000 \end{bmatrix},$$

$$V=\begin{bmatrix} 0.8666666667 & -4.2666666667 & 8.0000000000 & -4.2666666667 & 0.6666666667\\ 0.6666666667 & -2.4666666667 & 2.4000000000 & 1.3333333333 & -0.9333333333\\ 3.1800328864 & -12.5714190182 & 15.9862911541 & -3.1954642533 & -2.3994407690\\ 5.7320310842 & -23.1604784698 & 31.2568756177 & -9.5874584531 & -3.2409697790\\ 7.0624795575 & -28.7001489585 & 39.3380658942 & -12.9015637922 & -3.7988327010 \end{bmatrix}.$$

h	2^{-3}	2^{-4}	2^{-5}	2^{-6}
Order 3 method	4.74×10^{-7}	8.17×10^{-8}	1.18×10^{-8}	1.58×10^{-9}
p		2.54	2.79	2.90
Order 4 method	1.92×10^{-7}	1.46×10^{-8}	9.99×10^{-10}	6.40×10^{-11}
p		3.72	3.87	3.96

TABLE 1. The global error at the end of the interval of integration $[0, 2]$ for problem I.

4. Numerical experiments

In this section, the methods of orders $p = 3$ and $p = 4$, constructed in the subsections 3.3 and 3.4, are verified by some numerical experiments. We are going to confirm the expected orders and show the efficiency of the methods by their implementation on two well-known stiff IVPs. Here, the second derivative function, g, is obtained directly by $f_y f$.

Computational results are obtained by applying the methods on the following two stiff problems:

I. The non-linear stiff system of ODEs

$$\begin{cases} y_1' = -10004y_1 + 10000y_2^4, & y_1(0) = 1, \\ y_2' = y_1 - y_2(1 + y_2^3), & y_2(0) = 1, \end{cases}$$

with the exact solution $y_1(x) = \exp(-4x)$ and $y_2(x) = \exp(-x)$. This problem is stiff with approximately stiffness ratio 10^4 near to $x = 0$.

II. The Oregonator problem [27]

$$\begin{cases} y_1' = 77.27\left(y_2 + y_1(1 - 8.375 \times 10^{-6}y_1 - y_2)\right), & y_1(0) = 3, \\ y_2' = \frac{1}{77.27}(y_3 - (1 + y_1)y_2), & y_2(0) = 1, \\ y_3' = 0.161(y_1 - y_3), & y_3(0) = 2. \end{cases}$$

This is the famous chemical reaction with a periodic solution and an example of a stiff differential equation whose solutions change rapidly over many orders of magnitude.

In our numerical experiments for problem I, we integrate up to $\overline{x} = 2$. Numerical results for this problem are reported in Table 1. In this table,

x	y_i	A-$\overline{A}$-V-order3	A-$\overline{A}$-V-order4
90	y_1	1.003160059×10^0	1.003160066×10^0
	y_2	3.174467572×10^2	3.174460746×10^2
	y_3	1.029951843×10^0	1.029951485×10^0
180	y_1	1.033443057×10^0	1.033443131×10^0
	y_2	3.090095920×10^1	3.090089298×10^1
	y_3	1.028694646×10^0	1.028694710×10^0
270	y_1	1.502407022×10^0	1.502408659×10^0
	y_2	2.989869368×10^0	2.989862884×10^0
	y_3	1.408059791×10^0	1.408061045×10^0
360	y_1	1.001348484×10^0	1.001348484×10^0
	y_2	7.425667575×10^2	7.425667785×10^2
	y_3	6.403505527×10^0	6.403506359×10^0

TABLE 2. The results of Oregonator problem.

we have listed the norm of error $\|e_h(\overline{x})\|$ at the endpoint of integration $\overline{x}$ and numerical estimate to the order of convergence, p, computed by the formula

$$p = \frac{\log(\|e_h(\overline{x})\|/\|e_{h/2}(\overline{x})\|)}{\log(2)},$$

where $e_h(\overline{x})$ and $e_{h/2}(\overline{x})$ are errors corresponding to stepsizes h and $h/2$. To achieve the expected order, we used coefficients of these methods with 18 decimal digits. It is seen that the numerical estimation for the order coincides to the expected order for the implemented methods. Numerical results for the Oregonator problem are given in Table 2 and Figure 3.

5. **Conclusion**

Construction of SGLMs with RKS property, especially for the methods with a large number of r and s, requires the solution of large systems of polynomial equations of high degree for the unknown coefficients of the methods and hence it is a complicated task. In this paper, we introduced an special case of SGLMs, the so called A-$\overline{A}$-V methods, which

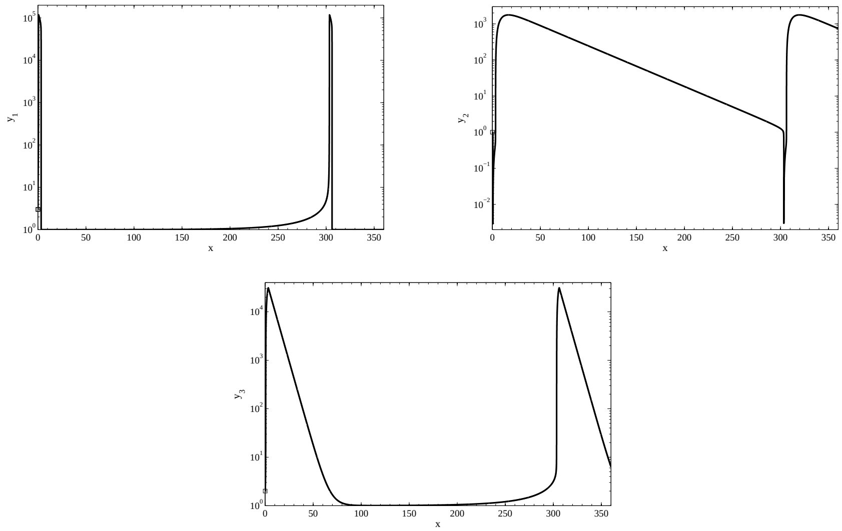

Figure 3. Solution components of the Oregonator problem vs. x.

makes the order conditions and the stability matrix of the methods to be simpler. The constructed methods are also L-stable so that, as it was shown in the numerical experiments, their implementation on stiff problems can be done successfully.

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