General linear methods for linear DAEs

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Abstract

For linear differential-algebraic equations (DAEs) with properly stated leading terms the property of being numerically qualified guarantees that qualitative properties of DAE solutions are reflected by the numerical approximations. In this case BDF and Runge-Kutta methods integrate the inherent regular ODE.
Here, we extend these results to general linear methods. We show how general linear methods having stiff accuracy can be applied to linear DAEs of index 1 and 2. In addition to the order conditions for ODEs, general linear methods for DAEs have to satisfy additional conditions.
As general linear methods require a starting procedure to start the integration we put special emphasis on finding suitable starting methods for index-2 DAEs.

1 Introduction

Differential algebraic equations (DAEs) arise naturally when modelling, among others, constrained mechanical systems, electrical circuits or chemical reaction kinetics. We are therefore interested in solving these equations efficiently and accurately. The reflexion of qualitative properties as well as stability questions are also important topics to address.
When modelling electrical circuits the main emphasis is not high accuracy, but the study of the numerical solution's qualitative behaviour becomes more important. It is well known that BDF methods may damp solutions undesirably. On the other hand, Runge-Kutta methods having good stability properties and high accuracy are often too expensive computationally.
General linear methods provide a unifying framework for multivalue and multistage methods. It is promising to study this large class of integration methods in order to find new methods that are suited for integrating DAEs with the required accuracy but being efficient and having good stability properties at the same time.
General linear methods for DAEs were studied in [3, 11]. The focus was on the development of methods and on the study of convergence for index-3 problems of Hessenberg type. However, DAEs arising in circuit simulation are not in

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Hessenberg form but are given with a properly stated leading term [9]. As a first step towards the application of general linear methods to DAEs of this type, we investigate linear DAEs with properly stated leading terms and index $\mu \in \{1, 2\}$. It is known that BDF and Runge-Kutta methods work satisfactory if the DAE is numerically qualified [7, 8]. It turns out that the same property property is relevant for integrating DAEs with general linear methods.
In section 2 we recall briefly the application of general linear methods to ordinary differential equations and introduce B-series for analysing these methods. The following section suggests a way of applying general linear methods to linear DAEs. The numerical solution obtained using this approach is studied in section 4. The last section presents some numerical experiments. Here we also compare different starting methods.

2 General linear methods and B-series

We consider a general linear method M given by the partitioned matrix

$$M = \left[\begin{array}{c|c} \mathcal{A} & \mathcal{U} \\ \hline \mathcal{B} & \mathcal{V} \end{array}\right], \qquad \begin{array}{ll} \mathcal{A} = (\mathfrak{a}_{ij}) \in L(\mathbb{R}^s), & \mathcal{U} = (\mathfrak{u}_{il}) \in L(\mathbb{R}^r, \mathbb{R}^s), \\ \mathcal{B} = (\mathfrak{b}_{kj}) \in L(\mathbb{R}^s, \mathbb{R}^r), & \mathcal{V} = (\mathfrak{v}_{kl}) \in L(\mathbb{R}^r). \end{array}$$

M is applied to ordinary differential equations $y'(t) = f\big(y(t), t\big)$ with right-hand side $f : \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}^m$ according to the scheme

$$Y'_{li} = f(Y_{li}, t_{l-1} + c_i h), \qquad i = 1, \dots, s, \tag{1a}$$

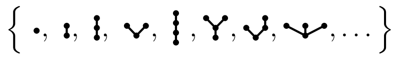
$$Y_l = h(\mathcal{A} \otimes I_m) Y'_l + (\mathcal{U} \otimes I_m) y^{[l-1]}, \tag{1b}$$

$$y^{[l]} = h(\mathcal{B} \otimes I_m) Y'_l + (\mathcal{V} \otimes I_m) y^{[l-1]}. \tag{1c}$$

$Y_{li} \in \mathbb{R}^m$, $i = 1, \dots, s$, are the stages calculated at $t_{li} = t_{l-1} + c_i h$ in step l. The corresponding stage derivatives are denoted as $Y'_{li} \in \mathbb{R}^m$. For compactness of notation we introduced the vectors

$$Y_l = \begin{pmatrix} Y_{l1} \\ \vdots \\ Y_{ls} \end{pmatrix} \in \mathbb{R}^{ms}, \quad Y'_l = \begin{pmatrix} Y'_{l1} \\ \vdots \\ Y'_{ls} \end{pmatrix} \in \mathbb{R}^{ms}, \quad y^{[l-1]} = \begin{pmatrix} y_1^{[l-1]} \\ \vdots \\ y_r^{[l-1]} \end{pmatrix} \in \mathbb{R}^{mr}.$$

The r quantities $y_k^{[l-1]} \in \mathbb{R}^m$, $k = 1, \dots, r$, represent some approximations calculated in step $l - 1$ that are passed on to the next step (see [1]).
General linear methods can be studied conveniently using B-series [5]. Let

$T = \Big\{$  $\Big\}, \qquad T^{\#} = T \cup \{\emptyset\}$

be sets of rooted trees and $\alpha : T^{\#} \to \mathbb{R}^n$ a vector valued function. The formal series

$$B\big(\alpha, y(t)\big) = \sum_{\tau \in T^{\#}} \frac{\alpha(\tau)}{\sigma(\tau)} h^{r(\tau)} \otimes F(\tau)\big(y(t)\big)$$

is called B-series for the elementary weight function α at $y(t)$ over a stepsize h. Here $F : T^{\#} \times \mathbb{R}^m \to \mathbb{R}^m$ denotes the elementary differentials corresponding to the ODE and $r(\tau)$ is the order of a given tree τ. $\sigma(\tau)$ measures the tree's symmetry. Note that we have $B\big(\alpha, y(t_0)\big) \in \mathbb{R}^{m \cdot n}$ for sufficiently small h.

We introduce the density $\gamma(\tau)$ of $\tau \in T^{\#}$ defined as the product over all vertices of the order of the subtree rooted at that vertex [1] and consider the special elementary weight functions

- $\mathbf{1}(\tau) = \begin{cases} 1 & , \ \tau = \emptyset \\ 0 & , \ \text{otherwise} \end{cases}$ with $B(\mathbf{1},\, y(t)) = y(t)$
- $E(\tau) = \dfrac{1}{\gamma(\tau)}$ with $B(E,\, y(t)) = y(t+h)$
- $C_i(\tau) = \dfrac{c_i^{r(\tau)}}{\gamma(\tau)}$ with $B(C_i,\, y(t)) = y(t + c_i h)$
- $D_k(\tau) = \begin{cases} \frac{r(\tau)!}{\gamma(\tau)} & , \ \text{if } r(\tau) = k \\ 0 & , \ \text{otherwise} \end{cases}$ with $B(D_k,\, y(t)) = h^k y^{(k)}(t)$

For a given weight function α we define

$$\alpha D : T^{\#} \to \mathbb{R}^n, \ \ \tau \mapsto (\alpha D)(\tau) = \begin{cases} 0 & , \ \text{if } \tau = \emptyset \\ \alpha(\tau_1) \cdots \alpha(\tau_l) & , \ \text{if } \tau = [\tau_1, \dots, \tau_l] \end{cases}$$

The product $\alpha(\tau_1) \cdots \alpha(\tau_l)$ is meant componentwise. Finally we assume that the input vector can be written as a B-series $y^{[l-1]} = B\big(S,\, y(t_{l-1})\big)$ with elementary weight function S.
We introduce the elementary weights

$$\eta : T^{\#} \to \mathbb{R}^s, \ \ \tau \mapsto \eta(\tau) = \mathcal{A}\big(\eta D\big)(\tau) + \mathcal{U} S(\tau)$$

$$\xi : T^{\#} \to \mathbb{R}^s, \ \ \tau \mapsto \xi(\tau) = \mathcal{B}\big(\eta D\big)(\tau) + \mathcal{V} S(\tau),$$

so that

$$Y_l = B\big(\eta,\, y(t_{l-1})\big) \qquad \text{and} \qquad y^{[l]} = B\big(\xi,\, y(t_{l-1})\big).$$

The general linear method M has order p relative to S if

$$\xi(\tau) = (ES)(\tau) \qquad \forall \ \tau \in T^{\#}, \ \ 0 \le r(\tau) \le p. \tag{2}$$

Here, ES is the elementary weight representing the composition of B-series

$$B\big(ES,\, y(t_{l-1})\big) = B\Big(S,\, B\big(E,\, y(t_{l-1})\big)\Big).$$

M has order p if there is an elementary weight function S such that (2) holds. q is said to be the stage order of M if it is the largest integer satisfying

$$\eta(\tau) = C(\tau) \qquad \forall \ \tau \in T^{\#}, \ \ 0 \le r(\tau) \le q, \tag{3}$$

where $C(\tau) = \big(C_1(\tau), \dots, C_s(\tau)\big)^T$.

3 The application of general linear methods to linear DAEs

Here we want to apply the general linear method M to linear differential-algebraic equations

$$A(t)\big(D(t)x(t)\big)' + B(t)x(t) = q(t), \qquad t \in \mathcal{I} \subset \mathbb{R}, \tag{4}$$

with properly stated leading terms [10, 12]. Be aware that we use the same letter q to denote the method's stage order and the DAE's right hand side. In (3) q is a number but in (4) it is a mapping so that there should be no confusion.

We replace (1a) by the linear system

$$A_{li}[DX]'_{li} + B_{li}X_{li} = q_{li}, \quad i = 1, \ldots, s. \tag{5a}$$

As in (5a) we often write $M_{li} = M(t_{li})$ for a mapping $t \mapsto M(t)$. Note that we reserve the y-notation for ODEs but use the x-notation for DAEs. The vector $[DX]'_l$ contains the numerical approximations $[DX]'_{li} \in \mathbb{R}^m$, $i = 1, \ldots, s$, to the derivatives $\big(D(t_{li})x(t_{li})\big)'$ satisfying

$$[DX]_l = h(\mathcal{A} \otimes I_m)[DX]'_l + (\mathcal{U} \otimes I_m)[Dx]^{[l-1]}. \tag{5b}$$

The components of $[DX]_l$ are the D parts $D(t_{li})X_{li}$ of the stages. The system (5a)-(5b) is solved for the stages X_{li}. However, for the trivial example $A = 0$, $B = I$ it is necessary that $\mathcal{A}$ is nonsingular. Since situations like this can occur as parts of larger problems we pose the following assumption.

(A1) Let $\mathcal{A}$ be nonsingular. Denote $\mathcal{A}^{-1} = (\tilde{\mathfrak{a}}_{ij})$.

After computing the stages the vector $[Dx]^{[l-1]}$ is updated as

$$[Dx]^{[l]} = h(\mathcal{B} \otimes I_m)[DX]'_l + (\mathcal{V} \otimes I_m)[Dx]^{[l-1]}. \tag{5c}$$

For practical methods the vector $y^{[l-1]}$ in (1c) containing incoming approximations is often chosen to be a Nordsieck vector, i.e. $y_k^{[l-1]}$ is an approximation to the scaled derivative $h^{k-1}y^{(k-1)}(t_{l-1})$, $k = 1, \ldots, r$. In general the solution x of (4) is continuous but only Dx is differentiable. Thus, in order to solve (4) using methods in Nordsieck form, one has to pass on information about the solutions D component only.
Information about the numerical solution x_l has to be calculated from the stage approximations X_{li}. Due to (5a) the stages satisfy the algebraic constraints. Therefore methods with stiff accuracy guarantee that the numerical solution $x_l = X_{ls}$ has the same property.

(A2) Let M be stiffly accurate, i.e. $\mathcal{A}_s = \mathcal{B}_1$, $\mathcal{U}_s = \mathcal{V}_1$ and $c_s = 1$.

Here, the subscript i denotes the i^{th} row of a given matrix.

In general the method M will be multi-valued so that a starting method is required to provide the initial input vector $[Dx]^{[0]}$. We write the starting method as a general linear method

$$\hat{M} = \left[\begin{array}{c|c} \hat{\mathcal{A}} & \hat{\mathcal{U}} \\ \hline \hat{\mathcal{B}} & \hat{\mathcal{V}} \end{array}\right]$$

with $\hat{\mathcal{U}} = e = (1, \ldots, 1)^T \in \mathbb{R}^s$ and $\hat{\mathcal{V}} \in \mathbb{R}^r$. Thus, $\hat{M}$ takes only the initial value as input but calculates r output values.

Before analysing the numerical solution obtained by (5) recall the definitions

$$\left.\begin{aligned}
G_0 &= AD, \quad B_0 = B \\
N_i &= \ker G_i, \\
S_i &= \{\, z \in \mathbb{R}^m \mid B_i z \in \operatorname{im} G_i \,\} = \{\, z \in \mathbb{R}^m \mid Bz \in \operatorname{im} G_i \,\}, \\
Q_i &= Q_i^2, \ \operatorname{im} Q_i = N_i, \ P_i = I - Q_i, \\
G_{i+1} &= G_i + B_i Q_i, \\
B_{i+1} &= B_i P_i - G_{i+1} D^- C_{i+1}' D P_0 \cdots P_i, \\
C_{i+1} &= D P_0 \cdots P_{i+1} D^-.
\end{aligned}\right\} \ i \geq 0$$

from [10, 12]. The matrices and subspaces are defined pointwise for $t \in \mathcal{I}$. Using this notation the exact solution of an index-2 DAE (4) can be written as

$$x = KD^- u - Q_0 Q_1 D^- (DQ_1 D^-)' u + (Q_0 P_1 + P_0 Q_1) G_2^{-1} q + Q_0 Q_1 D^- (D Q_1 G_2^{-1} q)' \tag{6}$$

where $K = I - Q_0 P_1 G_2^{-1} B$ and the component $u = DP_1 x$ satisfies the inherent regular ordinary differential equation

$$u' - \big(DP_1 D^-\big)' u + DP_1 G_2^{-1} B D^- u = DP_1 G_2^{-1} q. \tag{7}$$

4 Analysis of the numerical solution

Let (4) be a linear DAE with properly stated leading term and index $\mu \in \{1, 2\}$. Furthermore we assume (4) to be numerically qualified, i.e. DS_1 and DN_1 are constant subspaces. Let $\mathfrak{U}$ and $\mathfrak{V}$ be constant projectors onto DS_1 and DN_1 respectively.
As in [10] we have the decomposition

$$\mathbb{R}^n = \ker A(t) \oplus \operatorname{im} D(t) = \ker A(t) \oplus D(t) S_1(t) \oplus D(t) N_1(t) \quad \forall \ t \in \mathcal{I}.$$

The subspaces DS_1 and DN_1 are dealt with by the following lemma.

Lemma 4.1 *DP_1D^- and DQ_1D^- are projector functions satisfying*

(i) $DS_1 = \operatorname{im} DP_1 = \operatorname{im} DP_1 D^-, \qquad DN_1 = \operatorname{im} DQ_1 = \operatorname{im} DQ_1 D^-.$

If the subspaces DS_1 and DN_1 are constant and $\mathfrak{U}$, $\mathfrak{V}$ are constant projectors onto DS_1 and DN_1 respectively, then the following relations hold:

(ii) $DP_1 D^- \mathfrak{U} = \mathfrak{U}, \ DP_1 D^- \mathfrak{V} = 0, \ DQ_1 D^- \mathfrak{V} = \mathfrak{V}, \ DQ_1 D^- \mathfrak{U} = 0,$
(iii) $(DP_1 D^-)' \mathfrak{U} = 0, \ (DP_1 D^-)' \mathfrak{V} = 0, \ (DQ_1 D^-)' \mathfrak{V} = 0, \ (DQ_1 D^-)' \mathfrak{U} = 0.$

The proof can be found in [12]. Note that $u = DP_1 x \in \operatorname{im} DP_1 = DS_1 = \operatorname{im} \mathfrak{U}$, so that $u = \mathfrak{U} u$ and equation (6) reduces to

$$x = KD^- u + (Q_0 P_1 + P_0 Q_1) G_2^{-1} q + Q_0 Q_1 D^- (DQ_1 G_2^{-1} q)'. \tag{6'}$$

Similarly (7) reduces to

$$u' + DP_1 G_2^{-1} B D^- u = DP_1 G_2^{-1} q. \tag{7'}$$

4.1 Representation of the numerical solution

We apply the general linear method M to the DAE (4) and obtain the system

$$A_{li}[DX]'_{li} + B_{li}X_{li} = q_{li}, \quad i = 1,\dots,s, \tag{5a}$$

$$[DX]'_l = \frac{1}{h}(\mathcal{A}^{-1}\otimes I_m)\Big([DX]_l - (\mathcal{U}\otimes I_m)[Dx]^{[l-1]}\Big), \tag{5b}$$

$$[Dx]^{[l]} = h(\mathcal{B}\otimes I_m)[DX]'_l + (\mathcal{V}\otimes I_m)[Dx]^{[l-1]}. \tag{5c}$$

(5b) and (5c) yield

$$\begin{aligned}[Dx]^{[l]} &= (\mathcal{B}\mathcal{A}^{-1}\otimes I_m)[DX]_l + \big((\mathcal{V}-\mathcal{B}\mathcal{A}^{-1}\mathcal{U})\otimes I_m\big)[Dx]^{[l-1]}\\ &= (\mathcal{B}\mathcal{A}^{-1}\otimes I_m)[DX]_l + (\mathcal{M}_\infty\otimes I_m)[Dx]^{[l-1]}.\end{aligned}$$

Note that

$$\mathcal{M}_\infty = \mathcal{V} - \mathcal{B}\mathcal{A}^{-1}\mathcal{U} = \lim_{\|z\|\to\infty}\mathcal{M}(z)$$

is the method's stability matrix $\mathcal{M}(z) = \mathcal{V} + z\mathcal{B}(I - z\mathcal{A})^{-1}\mathcal{U}$ evaluated at infinity.
Provided that the initial input vector $[Dx]^{[0]}$ satisfies

$$[Dx]^{[0]}_k = \mathbf{u}^{[0]}_k + \mathbf{v}^{[0]}_k \in DS_1 \oplus DN_1, \qquad k = 1,\dots,r, \tag{8}$$

we can write

$$[Dx]^{[l]}_k = \mathbf{u}^{[l]}_k + \mathbf{v}^{[l]}_k \in DS_1 \oplus DN_1, \qquad k = 1,\dots,r, \tag{9}$$

for $l > 0$ with

$$\mathbf{u}^{[l]} = (\mathcal{B}\mathcal{A}^{-1}\otimes I_m)[DP_1X]_l + (\mathcal{M}_\infty\otimes I_m)\mathbf{u}^{[l-1]} \in DS_1, \tag{10a}$$

$$\mathbf{v}^{[l]} = (\mathcal{B}\mathcal{A}^{-1}\otimes I_m)[DQ_1X]_l + (\mathcal{M}_\infty\otimes I_m)\mathbf{v}^{[l-1]} \in DN_1. \tag{10b}$$

We will use the abbreviations

$$\mathbf{U}_{li} = D_{li}P_{1,li}X_{li}, \qquad \mathbf{V}_{li} = D_{li}Q_{1,li}X_{li}, \qquad i = 1,\dots,s.$$

Note that condition (8) is satisfied naturally by the starting method introduced in section 3.

To analyse the stage approximations calculated by (5a)-(5b) we apply the decoupling procedure from [10] to the numerical scheme and find that (5a) is equivalent to the system

$$\left.\begin{aligned}&(DP_1D^-)_{li}[DX]'_{li} + (DP_1G_2^{-1}BP_0P_1)_{li}X_{li}\\ &\qquad\qquad + (DP_1D^-)'_{li}D_{li}Q_{1,li}X_{li} = (DP_1G_2^{-1}q)_{li}\\ &-(Q_0Q_1D^-)_{li}[DX]'_{li} + (Q_0P_1G_2^{-1}BP_0P_1)_{li}X_{li}\\ &\quad + (Q_0P_1D^-)_{li}(DP_1D^-)'_{li}D_{li}Q_{1,li}X_{li} + Q_{0,li}X_{li} = (Q_0P_1G_2^{-1}q)_{li}\\ &\qquad\qquad D_{li}Q_{1,li}X_{li} = (DQ_1G_2^{-1}q)_{li}\end{aligned}\right\}$$

Due to lemma 4.1 this reduces to

$$\left.\begin{aligned}&(DP_1D^-)_{li}[DX]'_{li} + (DP_1G_2^{-1}BD^-)_{li}D_{li}P_{1,li}X_{li} = \big(DP_1G_2^{-1}q\big)_{li}\\ &-\big(Q_0Q_1D^-\big)_{li}[DX]'_{li} + \big(Q_0P_1G_2^{-1}BD^-\big)_{li}D_{li}P_{1,li}X_{li}\\ &\qquad\qquad + Q_{0,li}X_{li} = \big(Q_0P_1G_2^{-1}q\big)_{li}\\ &\qquad\qquad D_{li}Q_{1,li}X_{li} = \big(DQ_1G_2^{-1}q\big)_{li}\end{aligned}\right\} \tag{11}$$

From (5b) and (9) it follows that

$$
\begin{aligned}
(DP_1D^-)_{li}[DX]'_{li} &= (DP_1D^-)_{li}\frac{1}{h}\sum_{j=1}^{s}\tilde{\mathfrak{a}}_{ij}\Big(D_{lj}X_{lj} - \sum_{k=1}^{r}\mathfrak{u}_{jk}[Dx]_k^{[l-1]}\Big)\\
&= \big(DP_1D^-\big)_{li}\frac{1}{h}\sum_{j=1}^{s}\tilde{\mathfrak{a}}_{ij}\Big(D_{lj}P_{1,lj}X_{lj}+D_{lj}Q_{1,lj}X_{lj}-\sum_{k=1}^{r}\mathfrak{u}_{jk}\big(\mathbf{u}_k^{[l-1]}+\mathbf{v}_k^{[l-1]}\big)\Big)\\
&= \big(DP_1D^-\big)_{li}\frac{1}{h}\sum_{j=1}^{s}\tilde{\mathfrak{a}}_{ij}\Big(\mathbf{U}_{lj}+\mathbf{V}_{lj} - \sum_{k=1}^{r}\mathfrak{u}_{jk}\big(\mathbf{u}_k^{[l-1]}+\mathbf{v}_k^{[l-1]}\big)\Big).
\end{aligned}
$$

Again we apply lemma 4.1 and find that

$$
\begin{aligned}
(DP_1D^-)_{li}\mathbf{U}_{lj} &= (DP_1D^-)_{li}\,\mathfrak{U}\,\mathbf{U}_{lj} &&= \mathbf{U}_{lj}\\
(DP_1D^-)_{li}\mathbf{V}_{lj} &= (DP_1D^-)_{li}\,\mathfrak{V}\,\mathbf{V}_{lj} &&= 0\\
(DP_1D^-)_{li}\mathbf{u}_k^{[l-1]} &= (DP_1D^-)_{li}\,\mathfrak{U}\,\mathbf{u}_k^{[l-1]} &&= \mathbf{u}_k^{[l-1]}\\
(DP_1D^-)_{li}\mathbf{v}_k^{[l-1]} &= (DP_1D^-)_{li}\,\mathfrak{V}\,\mathbf{v}_k^{[l-1]} &&= 0
\end{aligned}
$$

and finally

$$
(DP_1D^-)_{li}[DX]'_{li} = \frac{1}{h}\sum_{j=1}^{s}\tilde{\mathfrak{a}}_{ij}\Big(\mathbf{U}_{lj} - \sum_{k=1}^{r}\mathfrak{u}_{jk}\mathbf{u}_k^{[l-1]}\Big) =: \mathbf{U}'_{li}.
$$

Note that

$$
\mathbf{U}'_l = \frac{1}{h}(\mathcal{A}^{-1}\otimes I_m)\Big(\mathbf{U}_l - (\mathcal{U}\otimes I_m)\mathbf{u}^{[l-1]}\Big)
$$

contains the method's approximations to the derivatives $\big(DP_1x\big)'_{li}$, $i = 1,\ldots,s$. Similarly one obtains

$$
(DQ_1D^-)_{li}[DX]'_{li} = \frac{1}{h}\sum_{j=1}^{s}\tilde{\mathfrak{a}}_{ij}\Big(\mathbf{V}_{lj} - \sum_{k=1}^{r}\mathfrak{u}_{jk}\mathbf{v}_k^{[l-1]}\Big) =: \mathbf{V}'_{li}
$$

implying that

$$
(Q_0Q_1D^-)_{li}[DX]'_{li} = (Q_0Q_1D^-)_{li}\mathbf{V}'_{li}.
$$

(11) can now be written as

$$
\left.\begin{aligned}
\mathbf{U}'_{li} + (DP_1G_2^{-1}BD^-)_{li}\mathbf{U}_{li} &= \big(DP_1G_2^{-1}q\big)_{li}\\
-(Q_0Q_1D^-)_{li}\mathbf{V}'_{li} + \big(Q_0P_1G_2^{-1}BD^-\big)_{li}\mathbf{U}_{li} + Q_{0,li}X_{li} &= \big(Q_0P_1G_2^{-1}q\big)_{li}\\
\mathbf{V}_{li} &= \big(DQ_1G_2^{-1}q\big)_{li}
\end{aligned}\right\} \quad (11')
$$

The numerical solution has therefore the representation

$$
\begin{aligned}
x_l = X_{ls} &= P_{0,ls}X_{ls} + Q_{0,ls}X_{ls}\\
&= D_{ls}^-\big(D_{ls}P_{1,ls}X_{ls} + D_{ls}Q_{1,ls}X_{ls}\big) + Q_{0,ls}X_{ls}\\
&= D_{ls}^-\mathbf{U}_{ls} + D_{ls}^-\mathbf{V}_{ls} + Q_{0,ls}X_{ls}\\
&= K_{ls}D_{ls}^-\mathbf{U}_{ls} + (P_0Q_1+Q_0P_1)_{ls}\big(G_2^{-1}q\big)_{ls} + (Q_0Q_1D^-)_{ls}\mathbf{V}'_{ls}.
\end{aligned} \quad (12)
$$

Remark 4.2 The decoupled system (11') provides the convergence of the general linear method applied to (4) on compact intervals $[t_0, T]$ as the stepsize tends to zero [13].

4.2 Order conditions for the DP_1 component

(10a) and (11') show that the components $\mathbf{U}_{li}$ of the stages X_{li} satisfy

$$\mathbf{U}'_{li} = -(DP_1G_2^{-1}BD^-)_{li}\mathbf{U}_{li} + (DP_1G_2^{-1}q)_{li} \tag{13a}$$

$$\mathbf{U}_l \ = h(\mathcal{A}\otimes I_m)\mathbf{U}'_l + (\mathcal{U}\otimes I_m)\mathbf{u}^{[l-1]}, \tag{13b}$$

$$\mathbf{u}^{[l]} = h(\mathcal{B}\otimes I_m)\mathbf{U}'_l + (\mathcal{V}\otimes I_m)\mathbf{u}^{[l-1]}. \tag{13c}$$

This is exactly the application of the general linear method M to the inherent regular ODE (7'), provided that in both cases the same initial input vector is used.
Denote by $u^{[0]}$ the input vector calculated by the starting method $\hat{M}$, when $\hat{M}$ is applied directly to the inherent regular ODE. Now repeat the decoupling procedure for the numerical result $[Dx]^{[0]} = \mathbf{u}^{[0]}+\mathbf{v}^{[0]}$ calculated by the starting method applied to the DAE.
It turns out that $u^{[0]}$ coincides with $\mathbf{u}^{[0]}$, so that the DP_1 component $\mathbf{U}_{ls} = \big(DP_1\big)_{ls}X_{ls}$ of the last stage computed by the general linear method M for $l > 0$ is exactly the numerical solution u_l when M is applied directly to the inherent regular ODE (7').

Even though we apply M to the DAE (4), the method internally deals with the inherent regular ODE (7') to solve for the DP_1 component.
In order to compute this component accurately, we therefore need to use methods M that realise high accuracy when applied to ODEs. The order conditions

$$(ES)(\tau) = \xi(\tau) = \mathcal{B}\big(\eta D\big)(\tau) + \mathcal{V}S(\tau), \qquad 0 \le r(\tau) \le p, \tag{2}$$

$$C(\tau) = \eta(\tau) = \mathcal{A}\big(\eta D\big)(\tau) + \mathcal{U}S(\tau), \qquad 0 \le r(\tau) \le q, \tag{3}$$

for general linear methods in the context of ODEs are also relevant when applying these methods to DAEs.

4.3 Order conditions for the DQ_1 component

From (11') we know that

$$\mathbf{V}'_l = \frac{1}{h}(\mathcal{A}^{-1}\otimes I_m)\Big(\mathbf{V}_l - (\mathcal{U}\otimes I_m)\mathbf{v}^{[l-1]}\Big)$$

where

$$\mathbf{V}_{li} = D_{li}Q_{1,li}X_{li} = \big(DQ_1G_2^{-1}q\big)_{li}$$

is exactly satisfied. (10b) implies

$$\begin{aligned}\mathbf{v}^{[l]} &= (\mathcal{B}\mathcal{A}^{-1}\otimes I_m)[DQ_1X]_l + \big((\mathcal{V}-\mathcal{B}\mathcal{A}^{-1}\mathcal{U})\otimes I_m\big)\mathbf{v}^{[l-1]} \\ &= (\mathcal{B}\mathcal{A}^{-1}\otimes I_m)[DQ_1G_2^{-1}q]_l + \big(\mathcal{M}_\infty\otimes I_m\big)\mathbf{v}^{[l-1]}.\end{aligned} \tag{14}$$

We analyse (14) by considering the ordinary differential equation

$$y'(t) = f(y,t) = \big(DQ_1G_2^{-1}q\big)'(t)$$

with exact solution $y(t) = (DQ_1G_2^{-1}q)(t)$.

Lemma 4.3 *The local error in the DQ_1 component $\mathbf{v}^{[l-1]}$ is of order $\tilde{q}$ (relative to the starting method S) if and only if*

$$\mathcal{B}\mathcal{A}^{-1}C(\tau) + \mathcal{M}_\infty S(\tau) = \big(ES\big)(\tau) \qquad \forall\ \tau \in T^{\#},\ 0 \le r(\tau) \le \tilde{q}. \tag{15}$$

Proof: (14) implies $\mathbf{v}^{[l]} = B\big(\mathcal{B}\mathcal{A}^{-1}C + \mathcal{M}_\infty S,\, y(t_{l-1})\big)$ but the exact value (relative to S) is given by $B\big(ES,\, y(t_{l-1})\big)$. □

Lemma 4.4 *Denote the order and stage order of the method M by p and q, respectively. Then* (15) *holds with $\tilde{q} = \min(p, q)$.*

Proof: For two elementary weight functions α and β write $\alpha =_k \beta$ if α and β agree for all trees τ with $0 \le r(\tau) \le k$. With this notation we have

$$\mathcal{B}\mathcal{A}^{-1}C + \mathcal{M}_\infty S =_q \mathcal{B}\mathcal{A}^{-1}\eta + \big(\mathcal{V} - \mathcal{B}\mathcal{A}^{-1}\mathcal{U}\big)S = \mathcal{B}(\eta D) + \mathcal{V}S =_p ES. \qquad \square$$

From lemma 4.4 it is clear that the DQ_1 component $\mathbf{v}^{[l]}$ is calculated with order p if M satisfies the condition

(A3) Let M have order and stage order equal to p.

It remains to show that the starting method $\hat{M}$ computes the DQ_1 component $\mathbf{v}^{[0]}$ of the initial input vector $[Dx]^{[0]}$ with order p as well. We have

$$\begin{aligned}
\mathbf{v}^{[0]} &= (\hat{\mathcal{B}}\hat{\mathcal{A}}^{-1} \otimes I_m)[DQ_1X]_0 \quad + \big((\hat{\mathcal{V}} - \hat{\mathcal{B}}\hat{\mathcal{A}}^{-1}\hat{\mathcal{U}}) \otimes I_m\big)D(t_0)Q_1(t_0)x_0 \\
&= (\hat{\mathcal{B}}\hat{\mathcal{A}}^{-1} \otimes I_m)[DQ_1G_2^{-1}q]_0 \ + (\hat{\mathcal{M}}_\infty \otimes I_m)\big(DQ_1G_2^{-1}q\big)(t_0) \\
&= B\big(\hat{\mathcal{B}}\hat{\mathcal{A}}^{-1}\hat{C} + \hat{\mathcal{M}}_\infty \mathbf{1},\, y(t_0)\big)
\end{aligned}$$

as $D(t_0)Q_1(t_0)x_0 = \big(DQ_1G_2^{-1}q\big)(t_0) = y(t_0)$ for every consistent initial value x_0. Since we intend to have

$$\mathbf{v}^{[0]} = B\big(S,\, y(t_0)\big) + \mathcal{O}(h^{p+1}),$$

condition (15) for the starting method now reads

$$\hat{\mathcal{B}}\hat{\mathcal{A}}^{-1}\hat{C}(\tau) + \hat{\mathcal{M}}_\infty \mathbf{1}(\tau) = S(\tau) \qquad \forall\ \tau \in T^{\#},\ 0 \le r(\tau) \le p. \tag{15'}$$

Remark 4.5 (15') applies to a starting method $\hat{M}$ that calculates the initial input vector at $t = t_0$. It is also possible to consider methods that actually take a step. Then condition (15) has to be satisfied for $\hat{M}$.

4.4 The main result

The results obtained in the previous sections are now summarised in the following theorem.

Theorem 4.6 *Let* (4) *be an index μ DAE, $\mu \in \{1, 2\}$, with a properly stated leading term. Let the subspaces $D(\cdot)S_1(\cdot)$ and $D(\cdot)N_1(\cdot)$ be constant, i.e.* (4) *is numerically qualified. For a general linear method M satisfying*

(A1) *$\mathcal{A}$ is nonsingular,*

(A2) *M is stiffly accurate,*

(A3) *M has order and stage order equal to p*

the difference between the exact solution $x(t_l)$ and the numerical solution x_l can be written as

$$x(t_l)-x_l = K_l D_l^- \big(u(t_l)-u_l\big) + (Q_0 Q_1 D^-)_l \Big\{ \big(DQ_1 G_2^{-1} q\big)'_l - [DQ_1 G_2^{-1} q]'_{ls} \Big\}.$$

u_l is exactly the general linear method's solution of the inherent regular ODE (7') and $[DQ_1 G_2^{-1} q]'_{ls}$ is M's approximation to $(DQ_1 G_2^{-1} q)'_l$.
Let S be the elementary weight function of a starting method $\hat{M}$ satisfying

$$(ES)(\tau) = \mathcal{B}\big(\eta D\big)(\tau) + \mathcal{V}S(\tau), \tag{2}$$

$$C(\tau) = \mathcal{A}\big(\eta D\big)(\tau) + \mathcal{U}S(\tau), \tag{3}$$

$$S(\tau) = \hat{\mathcal{B}}\big(\hat{\eta} D\big)(\tau) + \hat{\mathcal{V}}S(\tau), \tag{2'}$$

$$S(\tau) = \hat{\mathcal{B}}\hat{\mathcal{A}}^{-1}\hat{C}(\tau) + \hat{\mathcal{M}}_\infty \mathbf{1}(\tau), \tag{15'}$$

for $0 \le r(\tau) \le p$ then $[Dx]^{[l]} = \mathbf{u}^{[l]} + \mathbf{v}^{[l]}$ is calculated with local error of order $\mathcal{O}(h^{p+1})$.

<u>Proof:</u> Compare (6') and (12) to derive the representation of $x(t_l) - x_l$. (2') and (15') ensure that the initial input vector $[Dx]^{[0]} = \mathbf{u}^{[0]} + \mathbf{v}^{[0]}$ is calculated with order p. Finally, (2) and (3) guarantee that the calculation is carried on with the same order, as (2), (3) imply (15) (lemma 4.4). $\square$

Remark 4.7 Since the stage order is equal to the order p we get

$$\begin{aligned}
[DQ_1 G_2^{-1} q]'_l &= \frac{1}{h}(\mathcal{A}^{-1} \otimes I_m)\Big(\mathbf{V}_l - (\mathcal{U} \otimes I_m)\mathbf{v}^{[l-1]}\Big) \\
&= \frac{1}{h}(\mathcal{A}^{-1} \otimes I_m)\Big(B\big(C,\, y(t_{l-1})\big) - B\big(\mathcal{U}S,\, y(t_{l-1})\big)\Big) \\
&= \frac{1}{h}(\mathcal{A}^{-1} \otimes I_m) B\big(\mathcal{A}(\eta D),\, y(t_{l-1})\big) + \mathcal{O}(h^p) \\
&= \frac{1}{h} B\Big(D,\, B\big(\eta,\, y(t_{l-1})\big)\Big) + \mathcal{O}(h^p) \\
&= f\big(Y_l, t_{lc}\big) + \mathcal{O}(h^p).
\end{aligned}$$

The vector $f\big(Y_l, t_{lc}\big)$ contains the subvectors $f\big(Y_{li}, t_l + c_i h\big) = \big(DQ_1 G_2^{-1} q\big)'_{li}$, $i = 1, \ldots, s$, and we have

$$[DQ_1 G_2^{-1} q]'_{ls} = (DQ_1 G_2{}^{-}1q)'_l + \mathcal{O}(h^p)$$

for the local error of the derivative approximation. Since errors in this component are not propagated from step to step, the global error has the same order.

5 Numerical experiments

We consider the linear DAE $A(t)\big(D(t)x(t)\big)' + B(t)x(t) = q(t)$ taken from [6] given by the coefficients

$$\begin{pmatrix} 1 & 0 & 0 \\ \beta t{-}1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \left(\begin{pmatrix} 1 & 0 & 0 \\ 1{-}\beta t & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} x(t) \right)' + \begin{pmatrix} \alpha & -1 & -1 \\ \beta t(1{-}\beta t) & \alpha & -\beta t \\ 1{-}\beta t & 1 & 0 \end{pmatrix} x(t) = e^{-\alpha t} \begin{pmatrix} -1 \\ -\beta(1+t+\beta t^2) \\ -\beta t \end{pmatrix} \tag{16}$$

with constants α, $\beta \in \mathbb{R}$. (16) is a numerically qualified index-2 DAE with exact solution

$$x(t) = e^{-\alpha t} \begin{pmatrix} 1 \\ -1 \\ 2 \end{pmatrix}.$$

To solve (16) we use the general linear method proposed by Wright [14]

$$M = \left[\begin{array}{c|c} \mathcal{A} & \mathcal{U} \\ \hline \mathcal{B} & \mathcal{V} \end{array}\right] = \left[\begin{array}{ccc|ccc} \frac{1}{4} & 0 & 0 & 1 & 0 & \frac{-1}{32} \\ \frac{1}{6} & \frac{1}{4} & 0 & 1 & \frac{1}{12} & \frac{-1}{24} \\ \frac{1}{6} & \frac{1}{2} & \frac{1}{4} & 1 & \frac{1}{12} & \frac{-1}{24} \\ \hline \frac{1}{6} & \frac{1}{2} & \frac{1}{4} & 1 & \frac{1}{12} & \frac{-1}{24} \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -2 & 2 & 0 & 0 & 0 \end{array}\right], \quad c = \left(\tfrac{1}{4}, \tfrac{1}{2}, 1\right)^T.$$

M is in Nordsieck form, i.e. $y^{[l-1]}$ is an approximation to

$$\begin{pmatrix} y(t_{l-1}) \\ hy'(t_{l-1}) \\ h^2 y''(t_{l-1}) \end{pmatrix} = B\big(S, y_{l-1}\big), \quad S = \begin{bmatrix} \mathbf{1} \\ D \\ D_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \end{bmatrix}.$$

- M has strict stiff accuracy [14],
- M is in Nordsieck form,
- $\mathcal{A}$ is nonsingular,
- M has inherent Runge-Kutta stability [14].

To check the method's order and stage order we calculate

$$\mathcal{B}(\eta D) + \mathcal{V}S = \begin{bmatrix} 1 & 1 & \frac{1}{2} & \frac{37}{192} & \frac{37}{96} & \cdots \\ 0 & 1 & 1 & \frac{1}{2} & 1 & \cdots \\ 0 & 0 & 1 & \frac{3}{4} & \frac{3}{2} & \cdots \end{bmatrix}, \quad \eta = \begin{bmatrix} 1 & \frac{1}{4} & \frac{1}{32} & \frac{1}{128} & \frac{1}{64} & \cdots \\ 1 & \frac{1}{2} & \frac{1}{8} & \frac{7}{192} & \frac{7}{96} & \cdots \\ 1 & 1 & \frac{1}{2} & \frac{37}{192} & \frac{37}{96} & \cdots \end{bmatrix},$$

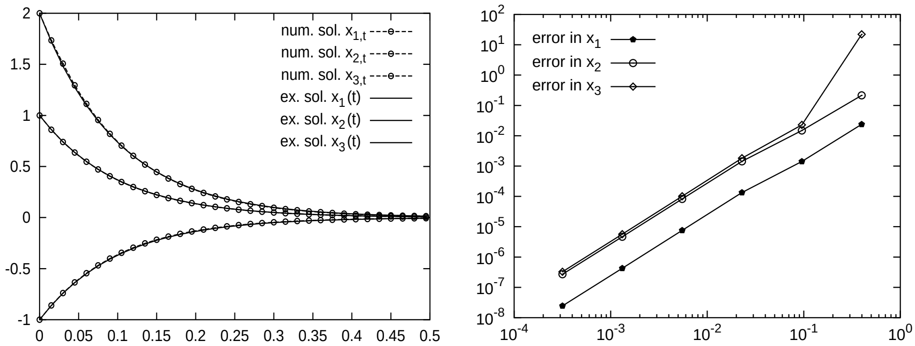
 

$$ES = \begin{bmatrix} 1 & 1 & \frac{1}{2} & \frac{1}{6} & \frac{1}{3} & \cdots \\ 0 & 1 & 1 & \frac{1}{2} & 1 & \cdots \\ 0 & 0 & 1 & 1 & 2 & \cdots \end{bmatrix}, \quad C = \begin{bmatrix} 1 & \frac{1}{4} & \frac{1}{32} & \frac{1}{384} & \frac{1}{192} & \cdots \\ 1 & \frac{1}{2} & \frac{1}{8} & \frac{1}{48} & \frac{1}{24} & \cdots \\ 1 & 1 & \frac{1}{2} & \frac{1}{6} & \frac{1}{3} & \cdots \end{bmatrix}.$$

It turns out that $\mathcal{B}(\eta D)(\tau) + \mathcal{V}S(\tau) = (ES)(\tau)$ and $\eta(\tau) = C(\tau)$ for all trees satisfying $0 \le r(\tau) \le 2$, i.e. the order and stage order is 2. From lemma 4.4 we know that condition (15) is satisfied for these trees as well:

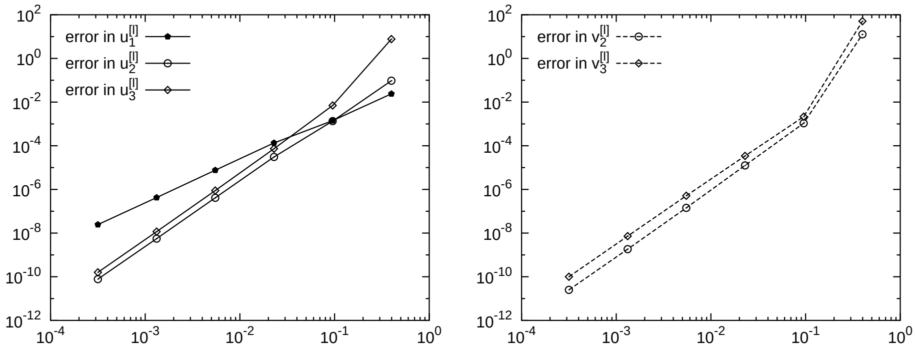
$$\mathcal{B}\mathcal{A}^{-1}C + \mathcal{M}_\infty S = \begin{bmatrix} 1 & 1 & \frac{1}{2} & \frac{1}{6} & \frac{1}{3} & \cdots \\ 0 & 1 & 1 & \frac{73}{144} & \frac{73}{72} & \cdots \\ 0 & 0 & 1 & \frac{31}{36} & \frac{31}{18} & \cdots \end{bmatrix}.$$

The numerical solution computed using exact input values is shown in figure 1(a). The order observed numerically is 2 as can be seen in figure 1(b).



(a) numerical solution for $h = 0.015$ (b) global error at $t = 0.5$ vs. stepsize

Figure 1: Numerical solution of (16) on the interval $[0, 0.5]$ using the exact initial Nordsieck vector. $x_0 = (1, -1, 2)^T$, $\alpha = 10$, $\beta = -20$.



(a) global error of $\mathbf{u}^{[l]}$ vs. stepsize (b) global error of $\mathbf{v}^{[l]}$ vs. stepsize ($\mathbf{v}_1^{[l]}$ is calculated exactly)

Figure 2: Global error of $[Dx]^{[l]} = \mathbf{u}^{[l]} + \mathbf{v}^{[l]}$

Figures 2(a) and 2(b) show the global error in the components $\mathbf{u}$ and $\mathbf{v}$. The order observed is 2 for $\mathbf{u}_1^{[l]}$ and even 3 for $\mathbf{u}_2^{[l]}$ and $\mathbf{u}_3^{[l]}$. Due to (15) with $\tilde{q}=p=2$ the local error in $\mathbf{v}^{[l]}$ is $\mathcal{O}(h^3)$. For linear DAEs it can be shown that the global error in this component has the same order as the local one. Thus we observe slope 3 in figure 2(b). As the $\mathbf{v}$ component is used for approximating the derivative $(DQ_1G_2^{-1}q)'$ the order of the derivative approximation remains 2.

In general it is not possible to start the calculation using exact input values represented by the elementary weight function S introduced earlier. One has to use a starting procedure to approximate the initial Nordsieck vector $[Dx]^{[0]}$.

We construct a starting method

$$\hat{M} = \left[\begin{array}{c|c} \hat{\mathcal{A}} & \hat{\mathcal{U}} \\ \hline \hat{\mathcal{B}} & \hat{\mathcal{V}} \end{array}\right]$$

by requiring $\hat{\mathcal{A}}$ to be singly diagonally implicit with eigenvalue $\frac{1}{4}$ and the stages Y_1, Y_2, Y_3 to be of order 1, 2 and 2 respectively [2]. These conditions determine $\hat{\mathcal{A}}$ uniquely. The entries of $\hat{\mathcal{B}}$ are chosen to ensure order 2 for this method when applied to ordinary differential equations.

$$\left[\begin{array}{ccc|c} \frac{1}{4} & 0 & 0 & 1 \\ \frac{1}{4}-\frac{1}{4}\sqrt{2} & \frac{1}{4} & 0 & 1 \\ \frac{1}{4}\sqrt{2} & \frac{-1}{4}-\frac{1}{4}\sqrt{2} & \frac{1}{4} & 1 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 4+2\sqrt{2} & -4-2\sqrt{2} & 0 \end{array}\right], \quad \hat{c} = \hat{\mathcal{A}}e = \begin{bmatrix} \frac{1}{4} \\ \frac{1}{4}(2-\sqrt{2}) \\ 0 \end{bmatrix} \tag{17}$$

Figure 3(a) shows that there arise serious problems when using this starting method for DAEs. The method is suited for ODEs as figure 3(b) shows order 2 behaviour for the $\mathbf{u}$ component. In spite of this the $\mathbf{v}$ component is integrated with order 1 only[1]. Note that although stages of order 2 were used exclusively to calculate the output, condition (15') does not hold for $\tilde{q} = 2$:

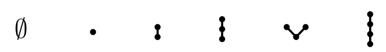
$$S - \hat{\mathcal{B}}\hat{\mathcal{A}}^{-1}\hat{C} - \hat{\mathcal{M}}_\infty\,\mathbf{1} = \begin{bmatrix} 0 & 0 & 0 & \cdots \\ 0 & 0 & -\frac{1}{8}+\frac{\sqrt{2}}{8} & \cdots \\ 0 & 0 & -\frac{\sqrt{2}}{2} & \cdots \end{bmatrix}.$$

Now consider the method

$$\hat{M}_2 = \left[\begin{array}{ccc|c} \frac{1}{4} & 0 & 0 & 1 \\ -\frac{1}{4} & \frac{1}{4} & 0 & 1 \\ \frac{3}{8} & -\frac{7}{8} & \frac{1}{4} & 1 \\ \hline 0 & 0 & 0 & 1 \\ \frac{1}{2} & 2 & -\frac{1}{2} & 0 \\ 8 & -12 & 4 & 0 \end{array}\right], \quad \hat{c} = \hat{\mathcal{A}}e = \begin{bmatrix} \frac{1}{4} \\ 0 \\ -\frac{1}{4} \end{bmatrix} \tag{18}$$

The stages Y_1 and Y_2 are of order 1 but Y_3 has order 2. This method has order 2 for ODEs and additionally satisfies (15') with the same order:

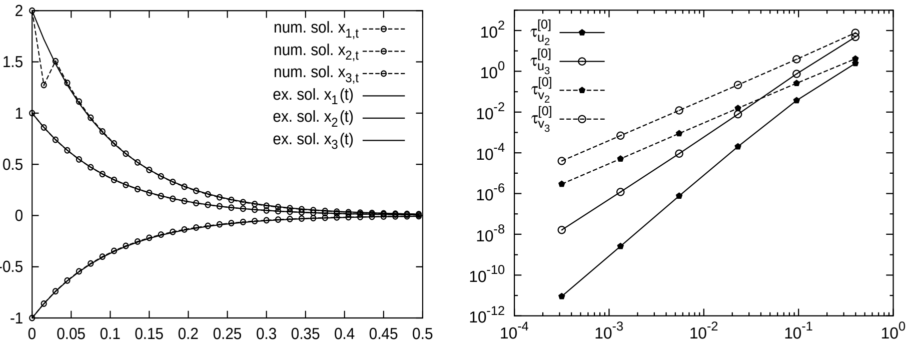
$$S - \hat{\mathcal{B}}(\hat{\eta}D) - \hat{\mathcal{V}}\mathbf{1} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \cdots \\ 0 & 0 & 0 & \frac{11}{64} & \frac{1}{16} & \frac{29}{256} \cdots \\ 0 & 0 & 0 & -\frac{11}{8} & -\frac{3}{4} & -\frac{27}{32} \cdots \end{bmatrix},$$



$$S - \hat{\mathcal{B}}\hat{\mathcal{A}}^{-1}\hat{C} - \hat{\mathcal{M}}_\infty\,\mathbf{1} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \cdots \\ 0 & 0 & 0 & \frac{1}{96} & \frac{1}{48} & 0 \cdots \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{192} \cdots \end{bmatrix}.$$

We conclude that not only $\mathbf{u}^{[0]}$ will be calculated with order 2 but also $\mathbf{v}^{[0]}$. Figure 4(b) confirms these results. Figure 4(a) shows that the time integration is now started correctly.

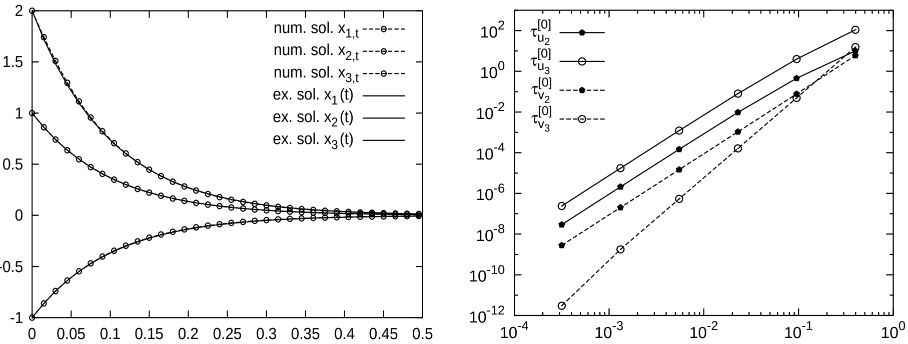
[1] Recall that the *local* error is plotted in figure 3(b), i.e. order p is represented by slope $p+1$.



(a) numerical solution for $h = 0.015$

(b) local error $\tau_{\mathbf{u}}^{[0]}$ and $\tau_{\mathbf{v}}^{[0]}$ vs. stepsize ($\mathbf{u}_1^{[0]}$ and $\mathbf{v}_1^{[0]}$ are calculated exactly)

Figure 3: Results for the starting method (17).



(a) numerical solution for $h = 0.015$

(b) local error $\tau_{\mathbf{u}}^{[0]}$ and $\tau_{\mathbf{v}}^{[0]}$ vs. stepsize ($\mathbf{u}_1^{[0]}$ and $\mathbf{v}_1^{[0]}$ are calculated exactly)

Figure 4: Results for the starting method (17).

Remark 5.1 The starting method suggested in (18) computes $\mathbf{v}_2^{[0]}$ with order 2 and $\mathbf{v}_3^{[0]}$ even with order 3. However, it uses information from the past as $c_3 = -\frac{1}{4} < 0$. It is possible to avoid this disadvantage. The starting method

$$\hat{M}_3 = \left[\begin{array}{ccc|c} \frac{1}{4} & 0 & 0 & 1 \\ -\frac{1}{4} & \frac{1}{4} & 0 & 1 \\ 1 & -\frac{1}{4} & \frac{1}{4} & 1 \\ \hline 0 & 0 & 0 & 1 \\ \frac{1}{3} & \frac{3}{4} & -\frac{1}{12} & 0 \\ \frac{4}{3} & -2 & \frac{2}{3} & 0 \end{array}\right], \qquad \hat{c} = \hat{\mathcal{A}}e = \begin{bmatrix} \frac{1}{4} \\ 0 \\ 1 \end{bmatrix}$$

performs equally well, but $\mathbf{v}_3^{[0]}$ is now of order 2.

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