Consistency of Krylov-W-methods in initial value problems *

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Abstract

We consider W-methods and ROW-methods for stiff initial value problems, where the stage equations are solved by Krylov techniques. By using a certain 'multiple Arnoldi process' over all stages the order of the fully-implicit one-step scheme is preserved with small Krylov dimensions. Bounds for these dimensions depending only on the actual W-method, not on the dimension of the ODE, are derived. Several example methods and possible extensions to other linearly-implicit methods are discussed and consequences for stepsize selection strategies are pointed out.

Key words. W-methods, Krylov subspaces, multiple Arnoldi process

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Short title: Consistency investigations

1 Introduction

For the numerical solution of stiff initial value problems

$$\begin{aligned} y'(t) &= f(t, y(t)) \\ y(t_0) &= y_0 \in \mathbb{R}^n, \end{aligned} \tag{1.1}$$

implicit or linearly implicit methods have to be used due to stability requirements. Rosenbrock-type schemes like ROW-methods (e.g. [9]) have shown to be very efficient solution methods for such problems. Their classical formulation is for autonomous problems only. The nonautonomous form of a s-stage ROW-method is given by [7], [16]

$$\begin{aligned} (I - h\gamma A)(k_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j) &= f_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j + h d_i f_t \qquad (1.2) \\ f_i &= f(t_m + c_i h, u_{m+1}^{(i)}) \\ u_{m+1}^{(i)} &= u_m + h \sum_{j=1}^{i-1} a_{ij} k_j \\ u_{m+1} &= u_m + h \sum_{i=1}^{s} b_i k_i \end{aligned}$$

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where

$$f_t = f_t(t_m, u_m), \quad d_i = \gamma + \sum_{j=1}^{i-1} \gamma_{ij}, \quad c_i = \sum_{j=1}^{i-1} a_{ij},$$

and

$$A = f_y(t_m, u_m). \tag{1.3}$$

This version has the same order for nonautonomous problems as the classical ROW-method for autonomous ones.

The scheme (1.2) is a W-method ([14]) if the partial derivative f_t is not used for nonautonomous problems. In this case, the matrix A need not be given by (1.3), an arbitrary matrix may be used instead. This choice, however, leads to an increase in the number of order conditions for the W-method. In connection with Krylov techniques we will consider W-methods which do use A given by (1.3). So, for autonomous problems they are identical to ROW-methods. But for nonautonomous problems their order is lower, in general, than that of the corresponding ROW-method. With respect to B-consistency W-methods can have favourable properties [17]. To both types of methods using (1.3) we will refer in the sequel as the *"underlying Rosenbrock-type method"*.

For large dimension n these methods (like any implicit method) spend most of their computing time for the evaluation of the Jacobian and for the solution of the linear stage equations. By using a standard iteration method like GMRES or Arnoldi's method for solving each individual stage equation this effort may be reduced. However, such a simple combination may waste effort by neglecting dependencies among the different systems. The Krylov-W-methods considered here re-use information from the Arnoldi process in earlier stages by replacing the matrix $A = f_y(t_m, u_m)$ in (1.2) by a low-rank approximation

$$T_i = Q_i Q_i^T A, \tag{1.4}$$

at stage i, where the orthogonal matrix $Q_i = \{q_1, ..., q_{\varkappa_i}\} \in \mathbb{R}^{n,\varkappa_i}$ is computed by a multiple Arnoldi process described in section 3. The important point here is that Q_i $(i > 1)$ is an extension of Q_{i-1}. The stage equation (1.2) then becomes

$$(I - h\gamma T_i)(k_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j) = f_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j + h d_i f_t =: w_i. \tag{1.5}$$

Since

$$(I - h\gamma Q_i Q_i^T A)^{-1} = I + h\gamma Q_i (I - h\gamma H_i)^{-1} Q_i^T A, \quad H_i = Q_i^T A Q_i \in \mathbb{R}^{\varkappa_i, \varkappa_i}, \tag{1.6}$$

the stage increment k_i may be computed by

$$\begin{aligned} k_i &= (I - h\gamma T_i)^{-1} w_i - \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j \\ &= [I + h\gamma Q_i (I - h\gamma H_i)^{-1} Q_i^T A] w_i - \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j, \end{aligned} \tag{1.7}$$

and we have to solve equations of dimension $\varkappa_i$ only. If, furthermore, the right-hand side w_i at the i-th stage belongs to the subspace

$$\mathcal{K}_i = \operatorname{span}\{q_1, ..., q_{\varkappa_i}\} = \operatorname{range} Q_i, \tag{1.8}$$

i.e.,

$$Q_i Q_i^T w_i = w_i, \tag{1.9}$$

the relation (1.7) simplifies further, leading to the following final form of the *Krylov-W-method*

$$\begin{aligned} k_i &= Q_i(I - h\gamma H_i)^{-1} Q_i^T w_i - \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j \\ w_i &= f_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j + h d_i f_t, \quad f_i = f(t_m + c_i h, u_{m+1}^{(i)}) \\ u_{m+1}^{(i)} &= u_m + h \sum_{j=1}^{i-1} a_{ij} k_j, \quad u_{m+1} = u_m + h \sum_{i=1}^{s} b_i k_i. \end{aligned} \tag{1.10}$$

Condition (1.9) will be satisfied by the multiple Arnoldi process described in section 3.

Since the computational effort of Arnoldi's method increases with $\varkappa^2 n$, the Krylov-W-method can be efficient for fairly low dimensions $\varkappa_i$ only. On the other hand, efficient stepsize selection strategies require certain minimum dimensions in order to have the main properties of the overall scheme, namely

- accuracy of the numerical solution, and
- stability of the numerical scheme.

Stability results for Krylov-W-methods using the classical Arnoldi process (with one start only) are given in [3], and for the multiple Arnoldi process in [12]. Numerical comparisons of a 3-stage W-method using a multiple Arnoldi process in Schmitt and Weiner [13] with the code VODPK of Byrne, Brown and Hindmarsh [4] for semidiscretized two-dimensional parabolic equations showed a good performance of this Krylov-W-method and confirmed good stability properties.

In this paper we will concentrate on the first item. We present a strategy for the modified multiple Arnoldi process that guarantees the Krylov-W-method to have the same order as the underlying Rosenbrock-type method and give upper bounds for Krylov dimensions that are sufficient for this property. The main result is, that the required dimensions $\varkappa_i$ do not depend on the dimension n of (1.1).

In section 2 we describe the multiple Arnoldi process for the computation of the matrices Q_i and H_i used in the Krylov-W-method (1.10) and prove some basic properties.

In section 3 we derive estimates for the consistency order of method (1.10). These rely heavily on certain features of the multiple Arnoldi process. For an underlying Rosenbrock-type method of order p we give a strategy that ensures order p for (1.10), as well.

Section 4 gives examples of methods, for both versions using f_t or not.

In section 5 we finally present an outline how these results can be adapted to other linearly-implicit methods, e.g. adaptive Runge-Kutta methods ([15], [16]) or the methods proposed by Hochbruck and Lubich [8].

Remark 1.1 1. Krylov techniques have also been used in multistep codes for the solution of the nonlinear systems of algebraic equations, see, for instance, Gear and Saad [6], Brown and Hindmarsh [1], Byrne [4]. Gallopoulos and Saad [5] and Saad [11] use Krylov approximations for linear differential equations with a constant coefficient matrix, where the integral representation of the solution is approximated.

2. An important consequence of our order results is, that the precise behaviour of the overall local error of the Krylov-W-method is known. Regardless of its magnitude it is guaranteed to behave as $\mathcal{O}(h^{p+1})$ for a method of order p. Hence, a classical stepsize selection strategy is justified. If the error of a Krylov method is controlled by a bound $ktol$ on residuals alone, the overall local error of the integration method contains two different components of the form $\mathcal{O}(h^{p+1}) + h \cdot ktol$. Here, a normal error control is justified for $ktol \ll \mathcal{O}(h^p)$ only.

3. When using Krylov approximations the exact computation of the Jacobian is not necessary, since it occurs in the form of matrix-vector products Av only, which can be approximated by a difference quotient

$$f_y(t_m, u_m)v = \frac{1}{\delta}(f(t_m, u_m + \delta v) - f(t_m, u_m)) + \mathcal{O}(\delta \|v\|^2). \tag{1.11}$$

Due to this feature these methods are often called “matrix-free”. In practice, δ is chosen in dependence on the machine precision and $\|u_m\|$, for instance. In our following investigations, we assume that the product $f_y v$ is evaluated exactly. However, it can easily be seen, that a consistency order p also holds with (1.11) if $\delta = \mathcal{O}(h^{p-1})$, at least. □

2 The multiple Arnoldi process

For the computation of the approximate solution u_{m+1} in (1.2) s systems of linear equations with the same coefficient matrix have to be solved. In the first stage

$$(I - h\gamma A)k_1 = w_1,$$

the classical Arnoldi method (cf. [10]) may be used to construct a sequence of orthonormal vectors $q_1, q_2, \ldots, q_{\varkappa_1}$, that constitute a basis for the Krylov subspace

$$\mathcal{K}(A, q_1, \varkappa_1) := \operatorname{span}\{q_1, ..., A^{\varkappa_1 - 1} q_1\},$$

i.e., $\mathcal{K}_1 = \mathcal{K}(A, q_1, \varkappa_1)$. This process mixes Krylov steps Aq_j (approximated by (1.11)) with Gram-Schmidt-orthogonalization

$$q_{j+1} = \frac{v}{\|v\|_2}, \quad v = (I - \sum_{l=1}^{j} q_l q_l^T) A q_j.$$

With these vectors q_j the matrices $Q_1 = (q_1, ..., q_{\varkappa_1})$ and $H_1 = Q_1^T A Q_1$ are formed. By using $q_1 = w_1/\|w_1\|$ (1.9) is satisfied, obviously. Note, that the matrix H_1 in (1.10) is in Hessenberg form.

For the later stages, $i > 1$, in (1.5) there are two basic alternatives in applying the Arnoldi method. The first is to treat all systems separately and start the iteration anew. The second is to keep the known information about A contained in Q_1 and T_1 and to continue the Arnoldi process in an appropriate way. In a recent paper [3], a first attempt was discussed, which simply continues the initial Arnoldi process. Although this method performs surprisingly well for different test problems, it has the drawback that w_i, $i \geq 2$, is, in general, no longer contained in the Krylov subspace range Q_i. This leads to an additional term of the form $(I - QQ^T)w_i$ in the residual which is difficult to handle in theoretical investigations and can lead to high Krylov dimensions in practical computations for some problems.

The multiple Arnoldi process re-uses information from previous stages but avoids dubious error contributions by incorporating the new right-hand sides w_i into the subspace range Q_i.

For our consistency investigations concerned with (1.5) we will consider the following algorithm which is a generalization of the one given in [13] for two right-hand sides. Here, the integers r_i, p_i^* are strategy parameters.

Multiple Arnoldi process (MAP):

First stage: (Classical Arnoldi process):

$$q_1 = v/\|v\|, \quad v = w_1,$$

$$q_{j+1} = v/\|v\|, \quad v = (I - \sum_{m=1}^{j} q_m q_m^T) A q_j, \quad j = 1, ..., \varkappa_1 - 1$$

$$\Rightarrow \quad \mathcal{K}_1 = \operatorname{span}\{q_1, ..., q_{\varkappa_1}\} = \mathcal{K}(A, q_1, \varkappa_1).$$

Stage $(i+1)$:

(I) Let $v := (I - \sum_{m=1}^{\varkappa_i} q_m q_m^T) w_{i+1}$. If $v = 0$, then we have $w_{i+1} \in \mathcal{K}_i$ and this Step is skipped.

$$\text{If } v \neq 0 \quad \text{then} \quad q_{\varkappa_i+1} = v/\|v\|$$
$$\Rightarrow \quad w_{i+1} \in \operatorname{span}\{q_1, ..., q_{\varkappa_i+1}\}$$

(II) Let $q_{l_1}, ..., q_{l_{r_{i+1}}}$ be those basis vectors from $\{q_1, ..., q_{\varkappa_i+1}\}$ (respectively, $\{q_1, ..., q_{\varkappa_i}\}$, if $v = 0$ in Step (I)), with

$$A q_{l_j} \notin \operatorname{span}\{q_1, ..., q_{\varkappa_i+1}\}.$$

At the second stage these are $q_{\varkappa_1}$ and $q_{\varkappa_1+1}$ in the general case. Most often is $r_{i+1} = i+1$, but we have $r_{i+1} < i+1$, if $w_j \in \mathcal{K}_{j-1}$ for some j, for instance, if the j-th stage of the W-method contains no new function evaluation.

Then, the next r_{i+1} basis vectors are defined by

$$q_{\varkappa_i+1+j} = v/\|v\|, \quad v = (I - \sum_{m=1}^{\varkappa_i+j} q_m q_m^T) A q_{l_j}, \quad j = 1, ..., r_{i+1}$$

$$\Rightarrow \quad A q_{l_j} \in \operatorname{span}\{q_1, ..., q_{\varkappa_i+1+j}\}.$$

(III) Further basis vectors $q_l,\ l > \varkappa_i + r_{i+1} + 1$, are computed by

$$q_{\varkappa_i+1+kr_{i+1}+j} = v/\|v\|, \quad j = 1, ..., r_{i+1},\ k = 1, ..., p^*_{i+1},$$

with

$$\begin{aligned} v =& (I - \sum_{m=1}^{\varkappa_i+kr_{i+1}+j} q_m q_m^T) A q_{\varkappa_i+(k-1)r_{i+1}+j+1}. \qquad (2.1) \\ \Rightarrow \quad & A q_{\varkappa_i+(k-1)r_{i+1}+j+1} \in \operatorname{span}\{q_1, ..., q_{\varkappa_i+1+kr_{i+1}+j}\}. \end{aligned}$$

(IV) Possible continuation by other strategies like the adaptive strategy of [13].

The strategy for choosing the sequence of basis vectors was designed to yield the following properties.

Lemma 2.1 *Due to (I) holds* $k_i \in \mathcal{K}_i$. $\square$

Lemma 2.2 *By (II), (III) it holds for every* $m \le \varkappa_i + p^*_{i+1} r_{i+1} + 1$ *that*

$$A q_m \in \operatorname{span}\{q_1, ..., q_\nu\}, \quad \nu = \max\{m + r_{i+1}, \varkappa_i + 1 + r_{i+1}\}. \quad \square \qquad (2.2)$$

A further important consequence is

Lemma 2.3 *Consider stage* i *and* $k \le i$. *If*

$$(T_i^l - A^l) w_k = 0 \quad \mathit{for} \quad l = 1, ..., q,$$

then the same is true for stage $j > i$:

$$(T_j^l - A^l) w_k = 0 \quad \mathit{for} \quad l = 1, ..., q.$$

Proof. The statement follows from

$$Q_j = \{Q_i, q_{\varkappa_i+1}, ..., q_{\varkappa_j}\} \quad \text{for} \quad j > i$$

by induction over l. $\blacksquare$

Remark 2.1 When applying the MAP, the matrices $H_i = Q_i^T A Q_i$ will no longer be in Hessenberg form. By using only steps (I) – (III), however, a generalized Hessenberg structure is maintained. There will be at most i additional subdiagonals in H_i. For example, at the second stage we have

$$H_2 = Q_2^T A Q_2 = \begin{pmatrix} * & * & & & & \cdots & * \\ * & * & & & & \cdots & \\ & \ddots & \ddots & & & & \vdots \\ & & * & * & & & \\ & & * & * & * & & \\ & & & \ddots & \ddots & \ddots & \vdots \\ & & & & * & * & * \end{pmatrix}$$

where the second subdiagonal starts in column $\varkappa_1$. $\square$

3 Consistency results

We will now construct conditions that guarantee the Krylov-W-method to have the same order as the underlying Rosenbrock-type method. Starting with the same (t_m, u_m) we compare stage increments $\widetilde{k}_i$ computed with the underlying Rosenbrock-type method and the values k_i from the Krylov-W-method. In the following all variables with a tilde correspond to the underlying Rosenbrock-type method (1.2) and those without tilde to the Krylov-W-method (1.5). We will first derive estimates of the form

$$k_i - \widetilde{k}_i = \mathcal{O}(h^{q_i})$$

and will assume, that f is sufficiently smooth. So, let

$$\beta_{ij} = a_{ij} + \gamma_{ij}, \quad \beta_i = \sum_{j=1}^{i-1} \beta_{ij}$$

and define

$$\begin{aligned} \mathcal{M}_i &= \{j : \ \beta_{ij} \neq 0\} \\ \mathcal{N}_i &= \{j : \ a_{ij} \neq 0 \text{ or } \gamma_{ij} \neq 0\} \\ \mathcal{B} &= \{j : \ b_j \neq 0\} \\ q_i^{(M)} &= \min_{j \in \mathcal{M}_i} q_j \\ q_i^{(N)} &= \min_{j \in \mathcal{N}_i} q_j . \end{aligned}$$

Theorem 3.1 *Assume*

$$\sum_{l=1}^{\infty} h^l \gamma^l (T_i^l - A^l) w_i = \mathcal{O}(h^{q_i^{(W)}}), \quad h \to 0. \tag{3.1}$$

Then, it holds

$$k_i - \widetilde{k}_i = \mathcal{O}(h^{q_i}) \quad \textit{with} \quad q_i = \min\{q_i^{(M)} + 1, q_i^{(N)} + 2, q_i^{(W)}\}. \tag{3.2}$$

Proof. For $h \to 0$ the stage increments k_i and $\widetilde{k}_i$ satisfy

$$\begin{aligned} k_i - \widetilde{k}_i &= \sum_{l=0}^{\infty} h^l \gamma^l T_i^l w_i - \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j - \sum_{l=0}^{\infty} h^l \gamma^l A^l \widetilde{w}_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} \widetilde{k}_j \\ &= f_i - \widetilde{f}_i + \sum_{l=1}^{\infty} h^l \gamma^l T_i^l w_i - \sum_{l=1}^{\infty} h^l \gamma^l A^l \widetilde{w}_i \\ &= f_i - \widetilde{f}_i + \sum_{l=1}^{\infty} h^l \gamma^l (T_i^l - A^l) w_i + \sum_{l=1}^{\infty} h^l \gamma^l A^l (w_i - \widetilde{w}_i). \end{aligned}$$

Taylor expansion shows

$$f_i - \widetilde{f}_i = hA_i \sum_{j=1}^{i-1} a_{ij}(k_j - \widetilde{k}_j), \quad A_i = A + \mathcal{O}(h)$$

and we obtain

$$\begin{aligned} k_i - \widetilde{k}_i =& hA_i \sum_{j=1}^{i-1} a_{ij}(k_j - \widetilde{k}_j) + \sum_{l=1}^{\infty} h^l \gamma^l (T_i^l - A^l) w_i \\ &+ \sum_{l=1}^{\infty} h^l \gamma^l A^l [hA_i \sum_{j=1}^{i-1} a_{ij}(k_j - \widetilde{k}_j) + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma}(k_j - \widetilde{k}_j)] \\ =& \sum_{l=1}^{\infty} h^l \gamma^l (T_i^l - A^l) w_i + hA \sum_{j=1}^{i-1} \beta_{ij}(k_j - \widetilde{k}_j) \\ &+ \mathcal{O}(h^2) \sum_{j=1}^{i-1} a_{ij}(k_j - \widetilde{k}_j) + \mathcal{O}(h^2) \sum_{j=1}^{i-1} \gamma_{ij}(k_j - \widetilde{k}_j) \\ =& \mathcal{O}(h^{q_i}). \quad \blacksquare \end{aligned}$$

This theorem allows to characterize the maximal order of the Krylov-W-method:

Corollary 3.1 *Let the underlying Rosenbrock-type method be of order p and let $q_i \geq p$ for all $i \in \mathcal{B}$. Then the Krylov-W-method (1.7) is of order p, too.* $\square$

Thus, the order depends on the parameters of the method and on the values $q_i^{(W)}$. The latter, $q_i^{(W)}$, grow with increasing dimension of the subspaces $\mathcal{K}_i = \{q_1, ..., q_{\varkappa_i}\}$. In fact, they are determined by the parameters p_i^* of the multiple Arnoldi process. From Lemma 2.2 we have the following relations:

1. From (I) follows $w_i \in \mathcal{K}_i$. This step increases the Krylov dimension by one.

2. (II) guarantees $(T_i - A)w_i = 0$, and the dimension is increased by r_i, where $r_i = i$, in general.

3. Step (III) with p_i^* sweeps guarantees the property

$$(T_i^l - A^l)w_i = 0, \quad l = 2, ..., p_i^* + 1. \tag{3.3}$$

   This raises the dimension by $p_i^* r_i$.

Evidently, the cost for steps (II) and (III) in the MAP increases strongly at higher stages. So we will try to minimize this effort by concentrating Arnoldi steps at the first stages and exploiting interrelations between the different right-hand sides w_i.

Lemma 3.1 *Let the following assumptions be satisfied. There exist $\delta_{ij} \in \mathbb{R}$, $\sigma_i \geq 1$ such that*

$$w_i = \sum_{j=1}^{i-1} \delta_{ij} w_j + \mathcal{O}(h^{\sigma_i}), \tag{3.4}$$

$$h^l(T_i^l - A^l)w_j = \mathcal{O}(h^q) \quad \text{for all } j \text{ with } \delta_{ij} \neq 0, \quad l = 1, ..., q, \tag{3.5}$$

$$h^l(T_i^l - A^l)w_i = \mathcal{O}(h^q) \quad \text{for } l = 1, ..., q - \sigma_i - 1. \tag{3.6}$$

Then,

$$h^l(T_i^l - A^l)w_i = \mathcal{O}(h^q) \quad \text{for } l = 1, ..., q, \tag{3.7}$$

und consequently

$$\sum_{l=1}^{\infty} h^l \gamma^l (T_i^l - A^l) w_i = \mathcal{O}(h^q).$$

Proof. For $l = 1, ..., q - \sigma_i - 1$ the statement is true by assumption.

For $l \geq q - \sigma_i$ we have with (3.4)

$$\begin{aligned} h^l(T_i^l - A^l)w_i &= \sum_{j=1}^{i-1} \delta_{ij} h^l (T_i^l - A^l) w_j + \mathcal{O}(h^q) \\ &= \mathcal{O}(h^q) \quad \text{by (3.5).} \quad \blacksquare \end{aligned}$$

This lemma yields a first upper bound for the subspace dimensions sufficient for maximal order of the Krylov-W-method.

Theorem 3.2 *Let the underlying Rosenbrock-type method be of order p and let steps (I) – (III) of the multiple Arnoldi process be executed with $p_i^* \geq \max\{0, p - \sigma_i - 2\}$.*

Then, the resulting Krylov-W-method is also of order p, using

$$\varkappa_1 \geq p, \quad \varkappa_i \geq \varkappa_{i-1} + (p_i^* + 1)i + 1. \tag{3.8}$$

Proof. By induction over the stages we show that

$$h^l(T_i^l - A^l)w_i = \mathcal{O}(h^p), \quad l = 1, ..., p.$$

For the first stage this follows directly from $\varkappa_1 = p$.

Now, let

$$h^l(T_k^l - A^l)w_k = \mathcal{O}(h^p), \quad l = 1, ..., p, \quad k \leq i - 1.$$

For the stage $i > 1$ we obtain from (3.3)

$$(T_i^l - A^l)w_i = 0 \text{ for } l = 1, ..., p - \sigma_i - 1,$$

which shows (3.6). By Lemma 3.1 we have

$$h^l(T_i^l - A^l)w_i = \mathcal{O}(h^p), \quad l = 1, ..., p,$$

and the statement follows immediately. ■

The dimensions (3.8) are upper bounds for the Krylov dimensions sufficient to obtain maximal order. Note, that they do not depend on the dimension n of the initial value problem.

However, (3.8) ist not optimal, since no special properties of the underlying Rosenbrock-type method, like $b_i = 0$, for instance, are exploited. In the following section we will consider specific methods and compute values for the exponents σ_i in (3.4).

4 Examples

In this section we discuss assumption (3.4) on the relation between different right hand sides w_i and show, that it is generally satisfied with $\sigma_i = 1$ or $\sigma_i = 2$ for realistic methods.

4.1 Methods using f_t

By Taylor expansion at (t_m, u_m) we get from (1.5) and Lemma 2.3

$$\begin{aligned} f_i &= f + c_i h f_t + c_i h f_y f + \mathcal{O}(h^2) \\ k_j &= f + h(\gamma + \beta_j)(f_t + f_y f) + \mathcal{O}(h^2) \end{aligned}$$

if $\varkappa_1 \geq 2$ and consequently

$$w_i = \frac{1}{\gamma} d_i f + h[\beta_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} \beta_j + d_i] f_t + h[\beta_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} \beta_j] f_y f + \mathcal{O}(h^2). \tag{4.1}$$

Since $d_1 = \gamma \neq 0$ we obtain for the second stage

$$w_2 = \frac{d_2}{d_1} w_1 + \mathcal{O}(h),$$

i.e. $\sigma_2 = 1$ in (3.4).

At stages $i \geq 3$ equation (4.1) shows

$$w_i = \delta_{i1} w_1 + \delta_{i2} w_2 + \mathcal{O}(h^2), \quad i \geq 3,$$

meaning (3.4) with $\sigma_i = 2$, if $\beta_2 \neq 0$ or $\beta_2 = \beta_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} \beta_j = 0$. In the first case the parameters are given by

$$\delta_{i2} = \frac{\beta_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} \beta_j}{\beta_2}, \quad \delta_{i1} = \frac{d_i - \delta_{i2} d_2}{d_1}.$$

With these properties, Theorem 3.2 can be refined for the widely used ROW-methods of order $p = 4$ using $p_2^* \geq 1$, $p_i^* \geq 0$. For classical methods with $s = p = 4$ the assumption $\beta_2 = \beta_{21} \neq 0$ is satisfied.

Theorem 4.1 *Let the underlying Rosenbrock-type method be of order $p = 4$ and $\beta_2 \neq 0$. Then the multiple Arnoldi process can be executed in such a way, that the Krylov-W-method with dimensions*

$$\varkappa_1 \geq 4, \quad \varkappa_2 \geq 9, \quad \varkappa_i \geq \frac{i^2}{2} + \frac{3i}{2} + 4 \quad \text{for} \quad i \geq 3$$

is of the same order $p = 4$. $\square$

Example 4.1 We consider the well-known ROW-method GRK4T [9] of order $p = 4$ in its nonautonomous form. The coefficients are given by

$$\begin{aligned}
\alpha_{21} &= 0.462, & \alpha_{31} &= -0.0815668168327, & \alpha_{32} &= 0.961775150166\\
\alpha_{41} &= \alpha_{31}, & \alpha_{42} &= \alpha_{32}, & \alpha_{43} &= 0\\
\gamma_{21} &= -0.270629667752, & \gamma_{31} &= 0.311254483294, & \gamma_{32} &= 0.00852445628482\\
\gamma_{41} &= 0.282816832044, & \gamma_{42} &= -0.457959483281, & \gamma_{43} &= -0.111208333333\\
b_1 &= 0.217487371653, & b_2 &= 0.486229037990, & b_3 &= 0\\
b_4 &= 0.296283590357, & \gamma &= 0.231
\end{aligned}$$

By the special choice of the coefficients α_{4i} only 3 function evaluations are required. Furthermore, with

$$\tilde{b}_1 = -0.717088504499, \quad \tilde{b}_2 = 1.77617912176, \quad \tilde{b}_3 = -0.0590906172617$$

a numerical solution of order 3 can be computed, allowing a step-size control by embedding. GRK4T gives excellent results for stiff systems (cf. [7]). Since $b_3 = 0$, by Lemma 3.1 it is only necessary to have $q_3 = 3$. So, instead of restrictions of Theorem 4.1, for GRK4T the following Krylov dimensions are sufficient

$$\varkappa_1 = 4, \quad \varkappa_2 = 9, \quad \varkappa_3 = 10, \quad \varkappa_4 = 15.$$

For autonomous systems holds

$$w_2 = (1 + \frac{\gamma_{21}}{\gamma}) f + h\beta_2 f_y f + \mathcal{O}(h^2).$$

With $\varkappa_1 = 4$

$$h^l (T_2^l - A^l) w_2 = \mathcal{O}(h^4)$$

follows for $l \geq 2$. So at the second stage step (I) and step (II) of the MAP are sufficient. Furthermore we can exploit the fact, that by the special coefficients $w_4 \in \mathcal{K}_3$ holds. This means that at the 4-th stage step (I) of the MAP is skipped and we have $r_4 = 3$. This reduces the dimensions to

$$\varkappa_1 = 4, \quad \varkappa_2 = 7, \quad \varkappa_3 = 8, \quad \varkappa_4 = 11. \qquad \square \tag{4.2}$$

To illustrate the theoretical results we have tested GRK4T with MAP with constant stepsize on the autonomous system

$$\begin{aligned} y_1' &= -0.1 y_1 \\ y_i' &= (y_{i-1} y_{i+2} - y_{i+1} y_i)^2 - 0.1 i y_i, \quad i = 2, \ldots, n-2 \\ y_{n-1}' &= -0.1(n-1) y_{n-1} \\ y_n' &= -0.1 n y_n \end{aligned}$$

with $n = 1000$. The initial values were taken from the exact solution

$$y_k(t) = e^{-0.1kt}$$

We have integrated the problem in the interval $[0, 1]$ with 50, 100, 150, ..., 1800 steps. Figure 4.1 shows the numerically obtained orders of convergence with the following sequences of Krylov dimensions:

$$4, 7, 8, 11 \text{ (GRK1)}, \qquad 3, 7, 8, 11 \text{ (GRK2)}, \qquad 4, 5, 6, 9 \text{ (GRK3)}$$

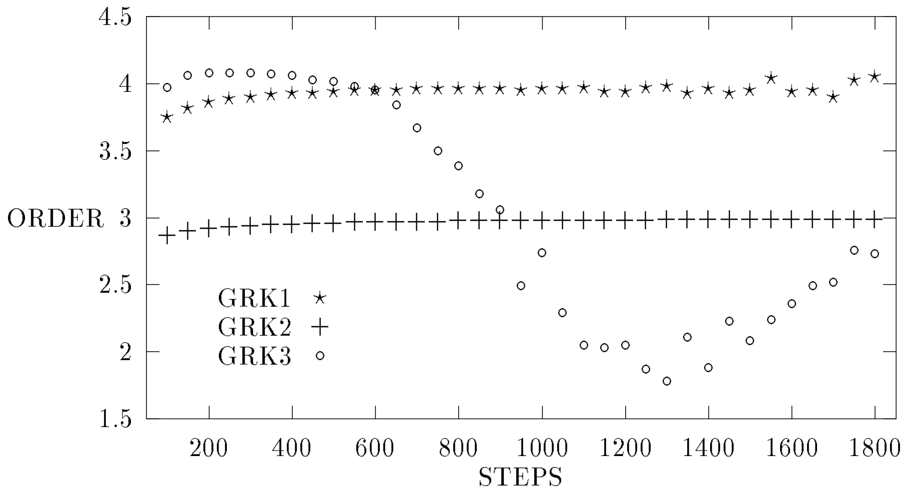

Figure 4.1: Numerically obtained order of convergence

GRK1 uses the minimal dimensions obtained in (4.2) and the results clearly reveal the claimed order 4. GRK2 shows the bound on $\varkappa_1$ to be sharp since the order drops to 3 if only the first dimension is lowered to $\varkappa_1 = 3$. For the later stages the results are not so decisive. The observed orders for GRK3, which uses inadequate dimensions only in the stages 2 to 4, show an irregular behaviour between 2 and 4.

4.2 Methods without f_t

There are special W-methods with favourable properties with respect to B-consistency. Compared with classical W-methods they are characterized by a higher number of stages, but a relatively small number of function evaluations [17]. These methods do not make use of the partial derivative f_t. So step (I) of the multiple Arnoldi process has not to be executed at all stages.

Analogously to (4.1) we obtain the expression

$$w_i = (1 + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma}) f + h(c_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} c_j) f_t + h(\beta_i + \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} \beta_j) f_y f + \mathcal{O}(h^2).$$

Obviously,

$$w_2 = (1 + \gamma_{21}/\gamma) w_1 + \mathcal{O}(h),$$

i.e. $\sigma_2 = 1$ in (3.4). For the third stage however, only $\sigma_3 = 1$ holds, in general, and order $\sigma_i = 2$ is possible only for $i \geq 4$.

Example 4.2 We consider the 3-stage W-method with 2 function evaluations

$$\begin{aligned}
(I - h\gamma T)k_1 &= f(t_m, u_m) \\
(I - h\gamma T)(k_2 - \frac{1}{\gamma}k_1) &= f(t_m + h, u_m + hk_1) - \frac{1}{\gamma}k_1 \\
(I - h\gamma T)(k_3 + (2\gamma - 3)k_1 + (1 - 2\gamma)k_2) &= f(t_m + h, u_m + hk_1) + (2\gamma - 3)k_1 + (1 - 2\gamma)k_2 \\
u_{m+1} &= u_m + \frac{h}{2}(k_1 + k_3),
\end{aligned}$$

$\gamma = 1 - \sqrt{2}/2$. With $T = A$ it is L-stable and has consistency order $p = 2$, the order of B-consistency for semi-linear systems is $q = 1$.

By Theorem 3.1 we need $q_1 = q_3 = 2$. For $\varkappa_1 \geq 2$ we have $q_1 = 2$. Since $\sigma_2 = 1$ it holds that

$$h(T_2 - A)w_2 = \mathcal{O}(h^2).$$

So, at the second stage we have only to execute step (I) of the MAP. Due to Lemma 2.2 and $f_2 = f_3$ we have $w_3 \in \mathcal{K}_2$. With $\sigma_3 = 1$ no increase of the Krylov dimension is required. Thus, already with

$$\varkappa_1 = 2, \quad \varkappa_2 = \varkappa_3 = 3$$

the Krylov-W-method has the order of consistency $p = 2$. $\square$

Remark 4.1 With these values $\varkappa_i$ the Krylov-W-method has the order of the underlying W-method. In practical computations also stability requirements have to be considered. Nevertheless, in numerical tests in [13] this 3-stage method produced good results with fairly low Krylov dimensions. $\square$

Example 4.3 In [17] an 8-stage W-method with 4 function evaluations of order $p = 3$ and B-consistency order $q = 2$ was constructed. For this method only b_1, b_5 and b_8 are different from zero and new function evaluations are executed at stages 1,2,4 and 6.

Therefore, the orders $q_1 = q_5 = q_8 = 3$ are required. For the other stages $q_i = 2$ is sufficient. The first condition, $q_1 = 3$, holds for $\varkappa_1 \geq 3$. At the second stage, due to the function evaluation, Arnoldi-Step (I) increases the dimension by one, yielding $\varkappa_2 \geq 4$. Without Step (II) we have by Lemma 3.1

$$\sum_{l=1}^{\infty} h^l \gamma^l (T_2^l - A^l) w_2 = \mathcal{O}(h^2),$$

since $\sigma_1 = 1$ and Theorem 3.1 yields $q_2 = 2$. At the third stage Step (I) is not necessary. Executing Step (II) increases the dimension to $\varkappa_3 \geq 6$ since $r_3 = 2$. This Step (II) ensures

$$(T_3 - A)w_3 = (T_3 - A)w_2 = 0.$$

By Lemma 3.1 and Lemma 2.3 follows from $\sigma_2 = \sigma_3 = 1$

$$\sum_{l=1}^{\infty} h^l \gamma^l (T_k^l - A^l) w_j = \mathcal{O}(h^3), \quad k \geq 3, \quad j = 2, 3.$$

At stages $i \geq 4$ this allows to apply Lemma 3.1 with $\sigma_i = 2$. As a consequence at these stages steps (II) and (III) can be skipped. The Krylov dimension has only to be increased at new function evaluations (step (I)). This yields as minimal dimensions

$$\varkappa_5 = \varkappa_4 = 7, \quad \varkappa_8 = \varkappa_7 = \varkappa_6 = 8. \qquad \Box$$

5 Other linearly-implicit methods

5.1 Adaptive Runge-Kutta methods

Another type of linearly-implicit Runge-Kutta methods is the class of adaptive Runge-Kutta methods. These methods have been derived by formally linearising the differential equation

$$y' = f(t, y) = Ay + g(t, y),$$

and approximating $g(t, y(t))$ by a polynomial $\tilde{g}(t)$. Then, the linear differential equation is solved exactly and the arising matrix-exponentials are approximated by rational functions [16]. Results for the application of Krylov techniques to this class can be found in [2].

In connection with Krylov methods one also can use the exponential form directly, since the computation of matrix functions takes place in a low-dimensional coordinate space. An s-stage adaptive Runge-Kutta method of this form is given by

$$\begin{aligned} u_{m+1}^{(i)} &= E_0(c_i hA) u_m + h \sum_{j=1}^{i-1} A_{ij}(c_i hA)[f_j - A u_{m+1}^{(j)}] \\ u_{m+1} &= E_0(hA) u_m + h \sum_{j=1}^{s} B_j(hA)[f_j - A u_{m+1}^{(j)}] \end{aligned} \tag{5.1}$$

with

$$f_j = f(t_m + c_j h, u_{m+1}^{(j)}), \quad u_{m+1}^{(1)} = u_m.$$

The matrix coefficients $A_{ij}(z)$, $B_j(z)$ are linear combinations of exponential functions $E_l(z)$ defined recursively by

$$\begin{aligned}E_0(z) &= \exp(z),\\ E_1(z) &= (E_0(z)-1)/z\\ E_{l+1}(z) &= (lE_l(z)-1)/z, \quad l=1,2,...\end{aligned} \tag{5.2}$$

Using (5.2) the methods can be reformulated in a form containing only one matrix function E_l at each stage. Here, a Krylov version of these methods is obtained by replacing the matrix argument A of E_l by a low-rank model $T_i = Q_i H_i Q_i^T$. Then, the function $E_l(c_i hA)$ may be computed by (see [3])

$$E_l(c_i hT_i) = Q_i E_l(c_i hH_i) Q_i^T.$$

If the matrices Q_i are again computed by a multiple Arnoldi process the earlier results on consistency can be adapted to this scheme. We will demonstrate this on the following example.

Example 5.1 For autonomous systems the method

$$\begin{aligned}u_{m+1}^{(2)} &= E_0(\frac{3}{4}hA)u_m + \frac{3}{4}hE_1(\frac{3}{4}hA)[f-Au_m]\\ u_{m+1} &= E_0(hA)u_m + hE_1(hA)\Big(\frac{19}{27}[f-Au_m] + \frac{8}{27}[f_2 - Au_{m+1}^{(2)}]\Big)\end{aligned}$$

is of order $p=4$ ([16]). It can be written in the form

$$\begin{aligned}u_{m+1}^{(2)} &= u_m + \frac{3}{4}hE_1(\frac{3}{4}hA)f_1\\ u_{m+1} &= u_m + hE_1(hA)\Big(\frac{19}{27}f_1 + \frac{8}{27}f_2 + \frac{8}{27}A(u_m - u_{m+1}^{(2)})\Big).\end{aligned} \tag{5.3}$$

In a Krylov approximation to this scheme, the Jacobian in E_1 is replaced by $T_i = Q_i H_i Q_i^T$, where Q_i is computed by the MAP using $w_1 = f_1$ and $w_2 = \frac{19}{27}f_1 + \frac{8}{27}f_2 + \frac{8}{27}A(u_m - u_{m+1}^{(2)})$. In the following discussion a tilde again corresponds to the method with exact Jacobian. With $w_1 = f_1$ and $\varkappa_1 = 4$ we have

$$u_{m+1}^{(2)} = \tilde{u}_{m+1}^{(2)} + \mathcal{O}(h^5).$$

This implies

$$f_2 = \tilde{f}_2 + \mathcal{O}(h^5)$$

and

$$\begin{aligned}\tilde{w}_2 &= \frac{19}{27}f + \frac{8}{27}\tilde{f}_2 + \frac{8}{27}A(u_m - \tilde{u}_{m+1}^{(2)})\\ &= \frac{19}{27}f + \frac{8}{27}f_2 + \frac{8}{27}A(u_m - u_{m+1}^{(2)}) + \mathcal{O}(h^5)\\ &= w_2 + \mathcal{O}(h^5).\end{aligned}$$

It follows

$$u_{m+1} - \tilde{u}_{m+1} = h(E_1(hT_2) - E_1(hA))w_2 + \mathcal{O}(h^5).$$

At the second stage Step (I) and Step (II) are performed. Since $w_2 = w_1 + \mathcal{O}(h)$, (i.e. $\sigma_1 = 1$) Step (III) of the MAP has to be executed with $p_2^* = 1$. This guarantees

$$(T^l - A^l)w_2 = 0, \quad l = 1, 2$$

and by Lemma 3.1

$$(E_1(hT_2) - E_1(hA))w_2 = \sum_{l=1}^{\infty} \frac{1}{(l+1)!} h^l (T_2^l - A^l) w_2 = \mathcal{O}(h^4).$$

Thus, with

$$\varkappa_1 \geq 4, \quad \varkappa_2 \geq 9$$

the Krylov version of this method has order $p = 4$, as well. $\square$

Remark 5.1 It is also possible to replace the Jacobian in the vector w_2 multiplied by $E_1(hA)$ of (5.3). This leads to the scheme

$$u_{m+1} = u_m + hE_1(hT_2)\Big(\frac{19}{27} f + \frac{8}{27} f_2 + \frac{8}{27} T_2(u_m - u_{m+1}^{(2)})\Big).$$

In this case one can compute $q_{\varkappa_1+1}$ by

$$q_{\varkappa_1+1} = v/\|v\|, \quad v = (I - \sum_{m=1}^{\varkappa_1} q_m q_m^T) f_2$$

and $E_1(hT_2)T_2(u_m - u_{m+1}^{(2)})$ in subspace coordinates by

$$E_1(hT_2)T_2(u_m - u_{m+1}^{(2)}) = Q_2 E_1(hH_2) H_2 Q_2^T (u_m - u_{m+1}^{(2)}).$$

By $u_m - u_{m+1}^{(2)} \in \mathcal{K}_1$ Step (II) of the Arnoldi process ensures

$$T_2(u_m - u_{m+1}^{(2)}) = A(u_m - u_{m+1}^{(2)}) + (T_2 - A)(u_m - u_{m+1}^{(2)}) = A(u_m - u_{m+1}^{(2)}).$$

Thus, the consistency result from Example 5.1 remains valid. $\square$

Remark 5.2 In general, there are two possibilities for Krylov approximations to these schemes. The matrix argument A in matrix-vector products $E_l(c_i hA)w_i$ may be replaced by either of the low-rank models $T_i = Q_i Q_i^T A$ and $T_i = Q_i Q_i^T A Q_i Q_i^T$. However, if the basis matrices Q_i are constructed by the MAP using these vectors w_i, both choices are equivalent, since

$$E_l(QQ^T A) = E_l(0) + Q E_l^{[1]}(Q^T A Q) Q^T A, \quad E_l^{[1]}(z) := (E_l(z) - E(0))/z,$$

cf. [3]. $\square$

5.2 The methods of Hochbruck and Lubich

Recently, Hochbruck and Lubich [8] proposed another generalization of W-methods for the use with Krylov techniques. For autonomous systems their method reads

$$
\begin{aligned}
k_i &= E_1(\gamma h A)\Big(f_i + hA\sum_{j=1}^{i-1}\gamma_{ij}k_j\Big)\\
u_{m+1} &= u_m + h\sum_{i=1}^{s} b_i k_i
\end{aligned}
\tag{5.4}
$$

with

$$f_i = f(u_m + h\sum_{j=1}^{i-1} a_{ij}k_j), \quad A = f_y(u_m).$$

By a discussion similar to that for adaptive Runge-Kutta methods, we consider replacing the Jacobian A in E_1 by $T_i = Q_i H_i Q_i^T$ and use again the relation

$$E_1(h\gamma T_i) = Q_i E_1(h\gamma H_i) Q_i^T$$

in the computation of the stage increments k_i if the basis matrices Q_i are constructed by the MAP with $w_i = f_i + hA\sum_{j=1}^{i-1}\gamma_{ij}k_j$, $i = 1,\dots,s$. We consider the stage increments $\widetilde{k}_i$ obtained with the full matrix A and k_i obtained with T_i. For $h \to 0$ we have

$$
\begin{aligned}
\widetilde{k}_i &= \sum_{l=0}^{\infty}\frac{1}{(l+1)!}(h\gamma A)^l \underbrace{\Big(\widetilde{f}_i + hA\sum_{j=1}^{i-1}\gamma_{ij}\widetilde{k}_j\Big)}_{\widetilde{w}_i}\\
k_i &= \sum_{l=0}^{\infty}\frac{1}{(l+1)!}(h\gamma T_i)^l \underbrace{\Big(f_i + hA\sum_{j=1}^{i-1}\gamma_{ij}k_j\Big)}_{w_i}.
\end{aligned}
\tag{5.5}
$$

Using the relations

$$
\begin{aligned}
f_i - \widetilde{f}_i &= hA_i\sum_{j=1}^{i-1} a_{ij}(k_j - \widetilde{k}_j), \quad A_i = A + \mathcal{O}(h)\\
w_i - \widetilde{w}_i &= hA\sum_{j=1}^{i-1}\beta_{ij}(k_j - \widetilde{k}_j) + \mathcal{O}(h^2)\sum_{j=1}^{i-1} a_{ij}(k_j - \widetilde{k}_j)
\end{aligned}
$$

we obtain

$$
\begin{aligned}
k_i - \widetilde{k}_i =& f_i - \widetilde{f}_i + hA\sum_{j=1}^{i-1}\gamma_{ij}(k_j - \widetilde{k}_j) + \sum_{l=1}^{\infty}\frac{1}{(l+1)!}h^l\gamma^l(T_i^l - A^l)w_i\\
&+ \sum_{l=1}^{\infty}\frac{1}{(l+1)!}(h\gamma A)^l(w_i - \widetilde{w}_i)\\
=& hA\sum_{j=1}^{i-1}\beta_{ij}(k_j - \widetilde{k}_j) + \mathcal{O}(h^2)\sum_{j=1}^{i-1} a_{ij}(k_j - \widetilde{k}_j) + \sum_{l=1}^{\infty}\frac{1}{(l+1)!}h^l\gamma^l(T_i^l - A^l)w_i.
\end{aligned}
$$

Changing the notations of Section 3 only slightly, the only difference being

$$\mathcal{N}_i = \{j : \ a_{ij} \neq 0\},$$

we finally arrive at

$$k_i - \tilde{k}_i = \mathcal{O}(h^{q_i^{(M)}+1}) + \mathcal{O}(h^{q_i^{(N)}+2}) + \mathcal{O}(h^{q_i^{(W)}}).$$

This gives

Corollary 5.1 *Let the method (5.4) be of order p and let $q_i \geq p$ for all $i \in \mathcal{B}$. Then the corresponding Krylov-W-method (5.4) is also of order p.* $\square$

By using Lemma 3.1 and the properties of the MAP better estimates for the orders $q_i^{(W)}$ are possible, again.

Remark 5.3 As in Remark 5.1, the Jacobian in w_i, (5.5), can be replaced by T_i. $\square$

6 Conclusions

The multiple Arnoldi process achieves two goals. It re-uses Krylov information from the different right hand sides of the stages of a Krylov-W-method and ensures that these right hand sides belong to the Krylov subspace. This simplifies the consistency investigations and allows to preserve the order of the underlying Rosenbrock-type method with moderate requirements on the selection strategy in the multiple Arnoldi process. We have derived estimates for the subspace dimensions required. An important aspect is, that these bounds on the subspace dimensions are independent of the dimension of the initial value problem. Thus, even for large problems the order of the underlying method is preserved with relatively small Krylov dimensions.

There are two practical consequences. The bounds on the subspace have to be taken into account if the maximal Krylov dimension is limited in practical computations. Another application is concerned with stepsize control. Since the order of a Krylov-W-method obeying the restrictions of Theorem 3.2 is the same as that of the underlying W-method, it is justified to use the same error estimation and stepsize prediction strategies.

By consistency considerations alone, it is advisable to concentrate dimension increases for the multiple Arnoldi process at lower stages. For stability reasons, however, further increases at higher stages may be necessary.

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