ON THE STABILITY OF APPROXIMATE TAYLOR METHODS FOR ODE AND THEIR RELATIONSHIP WITH RUNGE-KUTTA SCHEMES

A. BAEZA, S. BOSCARINO, P. MULET, G. RUSSO, AND D. ZORÍO

Abstract. In [Baeza et al., Computers and Fluids, 159, 156–166 (2017)] a new method for the numerical solution of ODEs is presented. This method can be regarded as an approximate formulation of the Taylor methods and it follows an approach that has a much easier implementation than the original Taylor methods, since only the functions in the ODEs, and not their high order derivatives, are needed. In this reference, the absolute stability region of the new methods is conjectured to be coincident with that of their exact counterparts. There is also a conjecture about their relationship with Runge-Kutta methods. In this work we answer positively both conjectures.

1. Introduction

In [1] we develop a numerical scheme consisting on an approximate formulation of Taylor methods for ODEs, akin to the scheme proposed by Zorío et. al. in [4] for hyperbolic conservation laws.

In [1] we show that high order schemes can be achieved with a computational cost that is competitive with that of Taylor methods, with the advantage that the approximate Taylor methods do not require the knowledge of higher order derivatives of the function in the ODE. In the cited reference there were the conjectures about the absolute stability region of the approximate methods coinciding with that of their exact counterparts and that they can be cast as Runge-Kutta schemes. We give here positive answers to both conjectures.

This paper is organized as follows: in Section 2 we recall the approximate Taylor methods and analyze their stability; in Section 3 we prove that the approximate Taylor methods are indeed Runge-Kutta methods.
2. Approximate Taylor methods

Without loss of generality, we consider initial value problems for systems of \( m \) autonomous ODEs for the unknown \( u = u(t) \):

\[
u' = f(u), \; u(0) = u_0,
\]

for nonautonomous systems can be cast as autonomous systems by considering \( t \) as a new unknown and by correspondingly inserting a new equation \( t' = 1 \) and initial condition \( t(0) = 0 \).

We aim to obtain approximations \( v_{h,n} \approx u(t_n) \) of the solution \( u \) of (1) on \( t_n = nh \), \( n = 0, \ldots \), with spacing \( h > 0 \). We use the following notation for time derivatives of \( u \):

\[
u^{(l)}_{h,n} = \frac{d^l u}{dt^l}(t_n).
\]

Our goal is to obtain an \( R \)-th order accurate numerical scheme, i.e., a scheme with a local truncation error of order \( R + 1 \), based on the Taylor expansion of the solution \( u \) from time \( t_n \) to the next time \( t_{n+1} \): \( \sum_{l=0}^{R} \frac{h^l}{l!} u^{(l)}_{h,n} + O(h^{R+1}) \).

To achieve this we aim to define approximations \( v^{(l)}_{h,n} \approx u^{(l)}_{h,n} \), with \( v^{(0)}_{h,n} = v_{h,n} \), by recursion on \( l \), such that

\[
v^{(l)}_{h,n} = u^{(l)}_{h,n} + O(h^{R+1-l}), \; l = 1, \ldots, R.
\]

Let us first briefly review how Taylor methods for (1) are obtained, by a simple scalar (\( m = 1 \)) example for third order accuracy (see, for instance, [3] for more details). The fact that \( u \) solves (1) implies that

\[
u'' = f'(u)u',
\]

\[
u''' = f''(u)(u')^2 + f'(u)u'',
\]

which yields

\[
u^{(1)}_{h,n} = u'(t_n) = f(u^{(0)}_{h,n})
\]

\[
u^{(2)}_{h,n} = u''(t_n) = f'(u^{(0)}_{h,n})u^{(1)}_{h,n}
\]

\[
u^{(3)}_{h,n} = u'''(t_n) = f''(u^{(0)}_{h,n})(u^{(1)}_{h,n})^2 + f'(u^{(0)}_{h,n})u^{(2)}_{h,n}.
\]

We have just proven that the definition

\[
v^{(1)}_{h,n} = f(v^{(0)}_{h,n})
\]

\[
v^{(2)}_{h,n} = f'(v^{(0)}_{h,n})v_{h,n}^{(1)}
\]

\[
v^{(3)}_{h,n} = f''(v^{(0)}_{h,n})(v_{h,n}^{(1)})^2 + f'(v_{h,n}^{(0)})v_{h,n}^{(2)},
\]

satisfies (2) with no error and that

\[
v_{h,n+1} = v_{h,n} + h v_{h,n}^{(1)} + \frac{h^2}{2} v_{h,n}^{(2)} + \frac{h^3}{6} v_{h,n}^{(3)}
\]

yields a third order scheme, the exact third order Taylor scheme.
It is readily seen that the $R$-th order Taylor methods applied to the equation $u' = \lambda u$ is given by

$$v_{h,n+1} = Q(h\lambda)v_{h,n}, \quad Q(x) = 1 + x + \frac{x^2}{2} + \cdots + \frac{x^R}{R!},$$

and, correspondingly, their region of absolute stability is

$$\{z \in \mathbb{C}: |Q(z)| \leq 1\}.$$

We propose in [1] an alternative solver, which is much less expensive for large $m, R$ and agnostic about the equation, in the sense that its only requirement is the knowledge of the function $f$. These solvers are based on the observation that approximations of (3) can be easily obtained by using finite differences of enough order, rather than using those expressions, that would only be exact for the analysis of the local truncation error.

For the sake of completeness we briefly describe here the scheme proposed in [1], along with the following auxiliary notation: For a function $u: \mathbb{R} \to \mathbb{R}^m$, we denote its sampling on the grid defined by a base point $a$ and grid space $h$ by

$$G_{a,h}(u): \mathbb{Z} \to \mathbb{R}^m, \quad G_{a,h}(u)_i = u(a + ih).$$

For naturals $p, q$, we denote by $\Delta_h^{p,q}$ the centered finite differences operator that approximates $p$-th order derivatives to order $2q$ on grids with spacing $h$, which, for any $u$ sufficiently differentiable, satisfies (see [4, Proposition 1] for the details):

$$|\Delta_h^{p,q}G_{a,h}(u) - u^{(p)}(a)| \leq K_{p,q} \max\{|u^{(p+2q)}(x)|: |x - a| \leq r_{p,q}h\}h^{2q},$$

for some $r_{p,q} \in \mathbb{N}$.

Given $v_{h,n}$, the approximations $v_{h,n}^{(k)} \approx u_{h,n}^{(k)}$ are defined by recursion on $k = 0, \ldots, R$ as follows:

$$\begin{align*}
v_{h,n}^{(0)} &= v_{h,n} \vspace{0.2cm} \\
v_{h,n}^{(1)} &= f(v_{h,n}) \vspace{0.2cm} \\
v_{h,n}^{(k+1)} &= \Delta_h^{k,\left\lfloor R-k \right\rfloor} \left(G_{0,h}(f(T_{h,n}^k))\right),
\end{align*}$$

where $T_{h,n}^k$ is the $k$-th degree approximate Taylor polynomial given by

$$T_{h,n}^k(\rho) = \sum_{l=0}^{k} \frac{v_{h,n}^{(l)}}{l!} \rho^l.$$

With all this notation, the proposed scheme is:

$$v_{h,n+1} = T_{h,n}^R(h) = \sum_{l=0}^{R} \frac{v_{h,n}^{(l)}}{l!} h^l = v_{h,n} + h \sum_{l=1}^{R} w_{h,n}^{(l)}, \quad w_{h,n}^{(l)} := \frac{v_{h,n}^{(l)}}{l!} h^{l-1}.$$

The following result is proven in [1] and it is a simplified adaptation of the corresponding result in [4].

**Theorem 1.** The scheme defined by (6) and (8) is $R$-th order accurate.

The following result, which corresponds to (4) and has been established for orders $R = 2, 3, 4$ in [1], is next proven for any $R$. 

STABILITY OF APPROXIMATE TAYLOR METHODS FOR ODE
Proposition 1. When applied to homogeneous linear systems \( u' = Au \), for an \( m \times m \) matrix \( A \), the scheme defined by (6) and (8) coincides with the exact Taylor method of the same order and therefore has the same stability region.

Proof. We consider \( f(u) = Au \), for an \( m \times m \) matrix \( A \), and first prove by induction on \( k \leq R \) that

\[
\nu_{h,n}^{(k)} = A^k v_{h,n},
\]

the case \( k = 0 \) being clear from (6). Assume \( k + 1 \leq R \), \( \nu_{h,n}^{(k)} = A^k v_{h,n} \) and use (6) and the linearity of \( \Delta_{h}^{k,q} \) to write

\[
\nu_{h,n}^{(k+1)} = \Delta_{h}^{k,q} (G_{0,h}(f(T_{h,n}^k))) = A \Delta_{h}^{k,q} (G_{0,h}(T_{h,n}^k)),
\]

for \( q = \left\lceil \frac{R-k}{2} \right\rceil \). Now (5), the fact that \( T_{h,n}^k \) is the \( k \)-th degree polynomial given in (7) and the induction hypothesis yield

\[
\Delta_{h}^{k,q} (G_{0,h}(T_{h,n}^k)) = (T_{h,n}^k)^{(k)}(0) = v_{h,n}^{(k)} = A^k v_{h,n},
\]

which, together with (10), therefore yields (9) for \( k + 1 \), thus concluding the proof by induction of (9).

Now, (8) immediately gives that

\[
\nu_{h,n}^{(k+1)} = Q(hA) \nu_{h,n}^{(k)},
\]

where \( Q \) is the \( R \)-degree polynomial in (4).

\[\Box\]

3. Relationship with Runge-Kutta schemes

In [1] it was conjectured that the \( R \)-th order approximate Taylor method could be cast as a Runge-Kutta method with \( R^2 + O(R) \) stages, which is asymptotically larger than the upper bound on the number of stages to achieve \( R \)-th order given in [2].

In this section we prove that the approximate Taylor methods are indeed Runge-Kutta schemes, by properly identifying their corresponding Butcher arrays. The following result, which is taken from [4], is at the foundation of this identification.

Theorem 2. For any \( p, q \in \mathbb{N} \), there exist \( \beta_{l}^{p,q} \), \( l = 0, \ldots, s := \left\lfloor \frac{p-1}{2} \right\rfloor + q \) such that

\[
\Delta_{h}^{p,q} v = \frac{1}{hp} \sum_{l=0}^{s} \beta_{l}^{p,q} (v_{h,l} + (-1)^p v_{h,-l})
\]

satisfies (5).

With the notation:

\[
f_{k,j} = f(T_{h,n}^k(jh)) = G_{0,h}(f(T_{h,n}^k))_j
\]

and (5) and (11), equation (6) yields:

\[
w_{h,n}^{(l+1)} = \frac{h^l}{(l+1)!} v_{h,n}^{(l+1)} = \frac{1}{(l+1)!} \sum_{i=-m_{l,R}}^{m_{l,R}} \gamma_{l,R}^i f_{l,i},
\]

where

\[
m_{l,R} = s_l \left\lceil \frac{R-l}{2} \right\rceil, \quad \gamma_{l,R}^i = (\text{sign}(i))^{\frac{l}{2}} \beta_{l}^{0,R},
\]

This equation is also valid for \( l = 0 \) if one takes \( m_{0,R} = 0 \) and \( \gamma_{0,R}^0 = 1 \):

\[
w_{h,n}^{(1)} = v_{h,n}^{(1)} = f(v_{h,n}) = f_{0,0}.
\]
From (12) and (13):

\[ f_{k,j} = f(T_{h,n}^k(jh)) = f(v_{h,n} + h \sum_{l=0}^{k-1} w_{h,n}^{(l+1)} j^{l+1}) \]

\[ = f(v_{h,n} + h \sum_{l=0}^{k-1} \frac{1}{(l+1)!} \sum_{i=-m_{l,R}}^{m_{l,R}} \gamma_{l,R}^{i,j} f_{l,i} j^{l+1}) \]

\[ f_{k,j} = f(v_{h,n} + h \sum_{l=0}^{k-1} \sum_{i=-m_{l,R}}^{m_{l,R}} \frac{j^{l+1} \gamma_{l,R}^{i,j}}{(l+1)!} f_{l,i}). \]

Notice that \( f_{k,0} = f_{0,0} = f(v_{h,n}) \forall k \). Therefore

\[ f_{k,j} = f(v_{h,n} + h \sum_{l=0}^{k-1} j^{l+1} g_{l,R}^{0,j} f_{0,0} + h \sum_{l=0}^{k-1} \sum_{i=-m_{l,R},i \neq 0}^{m_{l,R}} \frac{j^{l+1} \gamma_{l,R}^{i,j}}{(l+1)!} f_{l,i}). \]

Similarly, from (14), equation (8) reads:

\[ v_{h,n+1} = v_{h,n} + h \sum_{l=0}^{R-1} j^{l+1} g_{l,R}^{0,j} f_{0,0} + h \sum_{l=0}^{R-1} \sum_{i=-m_{l,R},i \neq 0}^{m_{l,R}} \frac{j^{l+1} \gamma_{l,R}^{i,j}}{(l+1)!} f_{l,i}). \]

Let us consider the subset of \( \mathbb{Z}^2 \):

\[ S_R = \{(0,0)\} \cup \{(l,i)/l \in \{1, R-1\}, i \in \{-m_{l,R}, \ldots, m_{l,R}\} \setminus \{0\} \}, \]

with size

\[ n_R := |S_R| = 1 + 2 \sum_{l=1}^{R-1} m_{l,R} \]

and with the lexicographical ordering given by the bijection

\[ I_R: S_R \rightarrow \{1, \ldots, n_R\}, \quad I_R(l,i) = \begin{cases} 0 & l = 0 \\ 2 + 2 \sum_{k<l} m_{k,R} + i + m_{l,R} & 0 < l < R, i < 0 \\ 1 + 2 \sum_{k<l} m_{k,R} + i + m_{l,R} & 0 < l < R, i > 0. \end{cases} \]

It can be proven that for \( l = 1, \ldots, R - 1 \):

\[ m_{l,R} = \begin{cases} \frac{R+1}{2} & R \text{ is even, } l \text{ is even} , \\ \frac{R-1}{2} & R \text{ is even, } l \text{ is odd} . \end{cases} \]

and from here and (13) that

\[ n_R = \begin{cases} 1 + (R - 1)^2 & R \text{ is odd} \\ 2 + (R - 1)^2 & R \text{ is even}. \end{cases} \]

We define the \( n_R \times n_R \) matrix \( A^{(R)} \) whose nonzero entries are given by:

\[ A^{(R)}_{I_R(k,j),I_R(l,i)} = \sum_{l=0}^{k-1} \frac{j^{l+1} \gamma_{l,R}^{i,j}}{(l+1)!} \]

\[ A^{(R)}_{I_R(l,i),I_R(l,i)} = \frac{j^{l+1} \gamma_{l,R}^{i,j}}{(l+1)!} \]

for \( k = 1, \ldots, R - 1, j = -m_{k,R}, \ldots, m_{k,R}, j \neq 0 \) and \( l = 1, \ldots, k - 1, i = -m_{l,R}, \ldots, m_{l,R}, i \neq 0. \)
We also define the $1 \times n_R$ vector $b^{(R)}$ as follows:

\begin{align}
  b_{I R(0,0)}^{(R)} &= \sum_{l=0}^{R-1} \frac{\gamma_{0,R}^{l,R}}{(l+1)!}, \\
  b_{I R(l,i)}^{(R)} &= \frac{\gamma_{i,R}^{l,R}}{(l+1)!}, \quad l > 0,
\end{align}

for $l = 1, \ldots, R - 1$, $i = -m_{l,R}, \ldots, m_{l,R}, i \neq 0$.

With this notation we have the following

**Theorem 3.**

1. The scheme defined by (6) and (8) is a $n_R$-stages Runge-Kutta scheme with Butcher array given by

   \[
   \begin{array}{c|c}
   c^{(R)} & A^{(R)} \\
   \hline
   b^{(R)}, & A^{(R)} \\
   \end{array}
   \]

   where $c_i^{(R)} = \sum_{j=1}^{i-1} A_{i,j}$.

2. $A^{(R)}$ is a block strictly lower $R \times R$ triangular matrix, with blocks of sizes $1, m_{1,R}, \ldots, m_{R-1,R}$.

3. $(A^{(R)})^R = 0$.

4. $\text{rank} A^{(R)} = R$.

**Proof.** Item 1 follows from (14), (15), (17) and (18).

Item 2 is clear from (17) and item 3 from this one. From (17)

\[ A_{I R(1,1)}^{(R)} = \gamma_{0,R}^{0,R} = 1, \]

therefore $A^{(R)}(:,1) \neq 0$.

From the proof of Theorem 2, for any $1 \leq l < R - 1$ there exists $i \in \{-m_{l,R}, \ldots, m_{l,R}\} \setminus \{0\}$ such that $\gamma_{i,R}^{l,R} \neq 0$. Therefore, for any $1 \leq k < R$, and any $j \in \{-m_{k,R}, \ldots, m_{k,R}\} \setminus \{0\}$ and any $1 \leq l < k$ there exists $i_t \in \{-m_{l,R}, \ldots, m_{l,R}\} \setminus \{0\}$ such that $\gamma_{i_t,R}^{l,R} \neq 0$.

From (17), $A_{I R(k,j),I R(l,i)}^{(R)} \neq 0$ and

\[ A_{I R(k,j),I R(l,i)}^{(R)} = A_{I R(k,j),I R(l,i)}^{(R)} \frac{\gamma_{i,R}^{l,R}}{\gamma_{i_t,R}^{l,R}}, \]

We have just proven that the columns $A^{(R)}(:, I R(l,i)), i = -m_{l,R}, \ldots, m_{l,R}, i \neq 0$, are proportional to $A^{(R)}(:, I R(l,i)) \neq 0$.

By the structure of the matrix,

$A^{(R)}(:,1), A^{(R)}(:, I R(1,i)), \ldots, A^{(R)}(:, I R(R-1,i))$

are linearly independent and all the columns of the matrix are proportional to one of these. Therefore, $\text{rank} A^{(R)} = R$. \hfill \Box

**Acknowledgments**

Antonio Baeza, Pep Mulet and David Zorío are supported by Spanish MINECO grants MTM 2014-54388-P and MTM2017-83942-P. D. Zorío is also supported by Fondecyt project 3170077. Giovanni Russo and Sebastiano Boscariino have been partially supported by Italian PRIN 2009 project “Innovative numerical methods for hyperbolic problems with application to fluid dynamics, kinetic theory, and computational biology”, Prot. No. 2009588FHJ.
References

[1] Baeza, A., Boscarino, S., Mulet, P., Russo, G. and Zorio, D.: Approximate Taylor methods for ODEs, Computers and Fluids, 159, 156–166 (2017).

[2] Butcher, J. C., 2008, Numerical methods for ordinary differential equations, 2nd Edition. John Wiley & Sons, Ltd., Chichester.

[3] Hairer, E. and Norsett, S. P. and Wanner, G., Solving ordinary differential equations. I, Springer Series in Computational Mathematics, 8, second edition, Springer-Verlag, 1993.

[4] Zorio, D., Baeza, A., Mulet, P.: An Approximate Lax-Wendroff-type procedure for high order accurate schemes for hyperbolic conservation laws. J. Sci. Comput., 71(1), 246–273 (2017).