Runge-Kutta Methods: Local error control does not imply global error control

J.S.C. Prentice
Department of Applied Mathematics,
University of Johannesburg,
South Africa

November 1, 2011

Abstract

We study the relationship between local and global error in Runge-Kutta methods for initial-value problems in ordinary differential equations. We show that local error control by means of local extrapolation does not equate to global error control. Our analysis shows that the global error of the higher-order solution is propagated under iteration, and this can cause an uncontrolled increase in the global error of the lower-order solution. We find conditions under which global error control occurs during the initial stages of the RK integration, but even in such a case the global error is likely to eventually exceed the user-defined tolerance.

Keywords: Runge-Kutta; Local error; Global error; Local extrapolation; Error control
MSC 2010: 65L05, 65L06, 65G99

1 Introduction

Runge-Kutta (RK) methods are the most popular choice of one-step methods for solving problems of the form

\[ \begin{align*}
    y' &= f(x,y) \\
    y(x_0) &= y_0
\end{align*} \]  

(1)

numerically. In the implementation of these methods, local error control via local extrapolation is the preferred choice of error control. It is known, however, that this form of error control does not amount to control of the global error. In this paper, we seek to give our own interpretation and discussion of this problem, including an analysis showing that global error control, if it does occur, is limited under RK iteration.
2 Relevant concepts

We now define local and global errors in RK methods formally, and study the propagation of local error in the implementation of an explicit RK method. We will also find the relationship between local and global error.

2.1 Runge-Kutta methods

The most general definition of a Runge-Kutta method [1] is

\[ k_p = f \left( x_i + c_p h, w_i + h \sum_{q=1}^{m} a_{pq} k_q \right) \quad p = 1, 2, ..., m \]

\[ w_{i+1} = w_i + h \sum_{p=1}^{m} b_p k_p \]  

Such a method is said to have \( m \) stages (the \( k_q \)). We note that if \( a_{pq} = 0 \) for all \( p \leq q \), then the method is said to be explicit; otherwise, it is known as an implicit RK method. The number of stages is related to the order of the method. The symbol \( w \) is used here and throughout to indicate the approximate numerical solution, whereas the symbol \( y \) will denote the true solution.

We denote an explicit Runge-Kutta method of order \( z \) (RKz) for solving (1) by

\[ w^z_{i+1} = w^z_i + h F^z (x_i, w^z_i) \]

where \( w^z_i \) denotes the numerical approximation to \( y(x_i) \) and \( F^z (x, y) \) is a function associated with the particular RKz method. Indeed, \( F^z \) is simply the linear combination of the stages for that particular method, as in

\[ F^z = \sum_{p=1}^{m} b_p k_p. \]

2.2 Local and global errors

We define the global error in a numerical solution at \( x_{i+1} \) by

\[ \Delta^z_{i+1} \equiv w^z_{i+1} - y_{i+1}, \]

and the local error at \( x_{i+1} \) by

\[ \varepsilon^z_{i+1} \equiv [y_i + h F^z(x_i, y_i)] - y_{i+1}. \]  

In the above, \( y_i \) denotes the true solution \( y(x_i) \), and similarly for \( y_{i+1} \). Note the use of the exact value \( y_i \) in the bracketed term in (3).

Previously, we have shown [2] that

\[ \Delta^z_{i+1} = \varepsilon^z_{i+1} + \alpha^z_i \Delta^z_i \]

\[ \alpha^z_i \equiv 1 + h F^z_y (x_i, \xi_i; h), \]  

2
where \( \xi_i \in (y_i, y_i + \Delta z_i) \). Equation (4) provides the relationship between local and global errors in RK\( \Delta z \). We will assume that \( \Delta_0 = 0 \) (i.e. the initial value is known exactly). We see that the global error at any node \( x_{i+1} \) is the sum of a local error term and a term incorporating the global error at the previous node. For convenience, we will drop the argument from \( F^z_y (x_i, \xi_i; h) \) in the remainder of the paper; its presence is implied.

For RK\( \Delta z \), it is well-known that 
\[
\varepsilon_{i+1}^{z} \propto h^{z+1} \\
\Delta_{i+1}^{z} \propto h^{z}.
\]

### 2.3 Local error estimation

Consider two RK methods of order \( z \) and \( z+1 \). Let \( w_{i+1}^{z} \) denote the approximate solution at \( x_{i+1} \) obtained with the order \( z \) method, and similarly for \( w_{i+1}^{z+1} \). Let the local error at \( x_{i+1} \) in the order \( z \) method be denoted by \( \varepsilon_{i+1}^{z} = \beta_{i+1}^{z} h^{z+1} \), and similarly for \( \varepsilon_{i+1}^{z+1} = \beta_{i+1}^{z+1} h^{z+2} \). Hence, with \( w_{i}^{z}, w_{i}^{z+1} = y_{i} \), we have
\[
w_{i+1}^{z} - w_{i+1}^{z+1} = \varepsilon_{i+1}^{z} - \varepsilon_{i+1}^{z+1} = \beta_{i+1}^{z} h^{z+1} - \beta_{i+1}^{z+1} h^{z+2} \\
\approx \beta_{i+1}^{z} h^{z+1}
\]
if \( h \) is sufficiently small. This gives
\[
\beta_{i+1}^{z} \approx \frac{w_{i+1}^{z} - w_{i+1}^{z+1}}{h^{z+1}}.
\]

### 2.4 Local error control

Once we have estimated the local error, we can perform error control. Assume that we require that the local error at each step must be less than a user-defined tolerance \( \delta \). Moreover, assume that, using stepsize \( h \), we find
\[
|\varepsilon_{i+1}^{z}| = |\beta_{i+1}^{z} h^{z+1}| \geq \delta.
\]
In other words, the magnitude of the local error \( \varepsilon_{i+1}^{z} \) exceeds the desired tolerance. We remedy the situation by determining a new stepsize \( h^{*} \) from
\[
|\beta_{i+1}^{z} \left[ h^{*}\right]^{z+1}| = \delta \Rightarrow h^{*} = \left( \frac{\delta}{|\beta_{i+1}^{z}|} \right)^{\frac{1}{z+1}}
\]
and we repeat the RK computation with this new stepsize. This, of course, gives
\[
x_{i+1} = x_{i} + h^{*}.
\]
This procedure is then carried out on the next step, and so on. Such form of error control is known as absolute error control. If the estimated error does not
exceed the tolerance, then no stepsize adjustment is necessary, and we proceed to the next step.

Often, we introduce a so-called ‘safety factor’ \( \sigma \), as in

\[
h^* = \sigma \left( \frac{\delta}{|\beta_{i+1}^z|^{1/\gamma}} \right)
\]

where \( \sigma < 1 \), so that the new stepsize is slightly smaller than that given by (6). This is an attempt to cater for the possibility that \( \beta_{i+1}^z \) may have been underestimated, due to the assumptions made in deriving (5). The choice of the value of \( \sigma \) is subjective, although a representative value is 0.8.

Note that because this error control algorithm is applied on each step, we could find that over the interval of integration we have step sizes of varying lengths. For this reason, it is appropriate to make the replacement

\[
h \rightarrow h_i \equiv x_{i+1} - x_i
\]

in (2).

2.5 Propagation of the higher-order solution

There is a very important point that must be discussed. The method for determining \( \beta_{i+1}^z \) hinged on the requirement \( w_i^z, w_{i+1}^{z+1} = y_i \). However, we only have the exact solution at the initial point \( x_0 \); at all subsequent nodes, the solution is approximate. How do we meet the requirement \( w_i^z, w_{i+1}^{z+1} = y_i \)?

In the case of local extrapolation, the answer is simple: simply use the higher-order solution \( w_i^{z+1} \) as input to generate both \( w_{i+1}^z \) (with the order \( z \) method), and \( w_{i+1}^{z+1} \) (with the order \( z + 1 \) method). In other words, we are assuming that \( w_{i+1}^{z+1} \) is accurate enough, relative to \( w_i^z \), to be regarded as the exact value, an assumption entirely consistent with the assumption made in deriving (5). This means that we determine the higher-order solution at each node, and this solution is used as input for both methods in computing solutions at the next node. The question of whether or not the global error that accumulates in the higher-order solution affects the calculation of \( \beta_{i+1}^z \) in (5) is addressed in the next section.

3 Analysis

3.1 The problem

Now, as per the last paragraph of the preceding section, assume that \( w_i^{z+1} \) is used to generate \( w_{i+1}^z \) and \( w_{i+1}^{z+1} \). Such value of \( w_{i+1}^z \) (and associated quantities)
will be denoted \( w^{z,z+1}_{i+1} \). Hence, we have

\[
\begin{align*}
\Delta^{z,z+1}_{i+1} &= \beta^{z}_{i+1} h^{z+1}_{i} + \alpha^{z,z+1}_{i} \Delta^{z+1}_{i} \\
&= \beta^{z}_{i+1} h^{z+1}_{i} + \Delta^{z+1}_{i} + h_{y} F^{z,z+1}_{y} \Delta^{z+1}_{i} \\
\Delta^{z+1}_{i+1} &= \beta^{z+1}_{i+1} h^{z+2}_{i} + \alpha^{z+1}_{i} \Delta^{z+1}_{i} \\
&= \beta^{z+1}_{i+1} h^{z+2}_{i} + \Delta^{z+1}_{i} + h_{y} F^{z,z+1}_{y} \Delta^{z+1}_{i}.
\end{align*}
\]

Thus,

\[
\begin{align*}
\Delta^{z,z+1}_{i+1} - \Delta^{z+1}_{i+1} &= \beta^{z}_{i+1} h^{z+1}_{i} + \Delta^{z+1}_{i} + h_{y} F^{z,z+1}_{y} \Delta^{z+1}_{i} \\
&= \beta^{z}_{i+1} h^{z+1}_{i} - \beta^{z+1}_{i+1} h^{z+2}_{i} + (F^{z,z+1}_{y} - F^{z+1}_{y}) h_{y} \Delta^{z+1}_{i} \\
&\approx \beta^{z}_{i+1} h^{z+1}_{i} + \Delta^{z+1}_{i}.
\end{align*}
\]

for small \( h_{y} \), because \( h_{y} \Delta^{z+1}_{i} = O(h^{z+2}_{i}) \). We see that the presence of global error in the higher-order solution does not affect the expression for \( \beta^{z}_{i+1} \) obtained under the assumption \( w^{z}_{i} = y_{i} \), particularly if \( h_{y} \) is small.

However, the expression for \( \Delta^{z,z+1}_{i+1} \) informs of a potential problem: we have

\[
\Delta^{z,z+1}_{i+1} = \beta^{z}_{i+1} h^{z+1}_{i} + \alpha^{z,z+1}_{i} \Delta^{z+1}_{i},
\]

where \( \Delta^{z+1}_{i} \) is the global error in \( w^{z}_{i} \). In (7), we see that a subtractive cancellation ensures that the \( \Delta^{z+1}_{i} \) term does not enter directly into the estimate for \( \beta^{z}_{i+1} \). Nevertheless, even if \( |\beta^{z}_{i+1} h^{z+1}_{i}| \leq \delta \), we could still have \( |\Delta^{z,z+1}_{i+1}| > \delta \), perhaps substantially so, if \( |\Delta^{z+1}_{i}| \) is large. Moreover, we should certainly expect that \( |\Delta^{z+1}_{i}| \) could become large under iteration (i.e. as \( i \) increases), since global error is essentially an accumulation of local errors. The point here is that, even if local error control is effective, the global error \( \Delta^{z,z+1}_{i+1} \) could become large, and could grow in an uncontrolled fashion.

### 3.2 Bounded global error via local error control?

Let us investigate the effect on the global error if local error control, via local extrapolation, is implemented. Consider the expression obtained previously for the global error at \( x^{i}_{i+1} \)

\[
\Delta^{z}_{i+1} = \varepsilon^{z}_{i+1} + \alpha^{z}_{i} \Delta^{z}_{i}.
\]

We assume \( \Delta^{0}_{0} = 0 \). If we have the exact value \( y_{i} \) at each node, then we have

\[
\Delta^{z}_{i+1} = \varepsilon^{z}_{i+1}
\]

at each node, so that the global error is equal to the local error. If the local error has been controlled (subject to tolerance \( \delta \)), we have

\[
\Delta^{z}_{i+1} \leq \delta
\]
which means that the global error satisfies the tolerance $\delta$.

However, as discussed previously, we do not have $y_i$ at each node. Rather, in the case of local extrapolation, where we have a higher-order solution available, and we propagate this higher-order solution, we have, from (8),

$$
\Delta^{z, z+1}_{i+1} = \beta^{z}_{i+1} h^{z+1} + \alpha^{z, z+1}_{i} \Delta^{z+1}_{i}
$$

$$
= \varepsilon^{z}_{i+1} + (1 + hF^{z+1}) \left( \varepsilon^{z+1}_{i} + \alpha^{z, z+1}_{i-1} \varepsilon^{z+1}_{i-1} + \ldots + \alpha^{z, z+1}_{i-2} \cdots \alpha^{z, z+1}_{1} \varepsilon^{z+1}_{1} \right)
$$

$$
= \varepsilon^{z}_{i+1} + \sum_{j=1}^{i} \varepsilon^{z+1}_{j} + O \left( h^{z+3} \right)
$$

$$
\lesssim \varepsilon^{z}_{i+1} + \sum_{j=1}^{i} \sigma^{z+2} \beta^{z+1}_{j} h^{z+2} = \sigma^{z+1} \beta^{z}_{i+1} h^{z+1} + \sigma^{z+2} \beta^{z+1} (x_i - x_0) h^{z+1},
$$

where $h$ is assumed to be the stepsize determined from (8) and we have included the safety factor $\sigma$ explicitly. For ease of analysis, we assume here a uniform stepsize $\bar{h}$. In the second last line, we assume that, since $\varepsilon^{z}_{i+1} \leq \delta$ and $\varepsilon^{z+1}_{j} \ll \varepsilon^{z}_{j}$ (the fundamental assumption in local extrapolation), we must have $\varepsilon^{z+1}_{j} \leq \delta$.

We denote the average value of $\beta^{z}_{i+1}$ on $[x_0, x_i]$ by $\bar{\beta}^{z+1}_{i+1}$, and we use $ih = x_i - x_0$. Now, assuming $\bar{\beta}^{z+1}_{i+1} (x_i - x_0) h^{z+1} < \delta$ (see the Appendix), we have

$$
\left| \Delta^{z, z+1}_{i+1} \right| \approx \sigma^{z+1} \delta + \sigma^{z+2} \left| \bar{\beta}^{z+1}_{i+1} (x_i - x_0) \right| h^{z+1}
$$

$$
\lesssim \sigma^{z+1} \delta + \sigma^{z+2} \delta
$$

$$
= \sigma^{z+1} + \sigma^{z+2} \delta.
$$

(10)

It is easily confirmed that for $\sigma = 0.8$, we have $(\sigma^{z+1} + \sigma^{z+2}) < 1$ for $z \geq 2$. This means that

$$
\left| \Delta^{z, z+1}_{i+1} \right| < \delta
$$

for these values of $\sigma$ and $z$, which suggests that the global error, like the local error, satisfies the user-defined tolerance. In other words, propagation of the higher-order solution in local error control via local extrapolation, has resulted in control of the global error, although the significance of the safety factor in deriving this result should be clear. Most importantly, the above result holds only if the assumptions made here are true; if they are not, then $\left| \Delta^{z, z+1}_{i+1} \right|$ is probably greater than $\delta$. For this reason, we say that the global error is possibly bounded, but this is not guaranteed. We should appreciate that such a bounding of the global error is a beneficial by-product of local error control, and is not the designated objective.

The most important assumption made above is

$$
\left| \bar{\beta}^{z+1}_{i+1} (x_i - x_0) \right| h^{z+1} < \delta.
$$
In the Appendix, we show that this is, in fact, a consequence of the condition
\[ |\beta_{i+1}^z| h^{z+1} > i |\bar{\beta}_{i+1}^{z+1}| h^{z+2}. \] (11)

If this condition is violated, then the assumption does not hold. It is worth examining this condition in closer detail: the factor \( i \) represents iteration number. It is quite reasonable to assume that there exists a value of \( i \) such that, for the given values of \( \bar{\beta}_{i+1}^{z+1} \) and \( h \), we will have
\[ |\beta_{i+1}^z| h^{z+1} < i |\bar{\beta}_{i+1}^{z+1}| h^{z+2}. \]

In other words, eventually the RK iterative process will cause (11) to be violated. This means that sooner or later the global error will exceed the imposed tolerance, despite local error control, and that the bounding of the global error will be ‘short-lived’, so to speak.

We also note that our assumption of a uniform stepsize is reasonable if the stepsize does not vary considerably; nevertheless, in reality it may do so, which would also compromise the validity of (11).

4 Comments

Some comments are appropriate:

1. We are not restricted to using a method of order \( z + 1 \) as the higher-order method in local extrapolation. Any method of order \( z + r, r \geq 1 \) can be used. Our analysis and results are essentially unchanged, save for (10), which becomes
\[ |\Delta_{i+1}^{z+r+1}| \leq (\sigma^{z+1} + \sigma^{z+r+1}) \delta. \]
The value of \( r \) here will influence the value of the safety factor \( \sigma \) for which the coefficient is less than unity.

2. Our analysis clearly shows that global error control cannot be achieved through local extrapolation. Global error control is usually achieved through reintegration - estimating the global error after local extrapolation, and then redoing the computation on the entire interval of integration with a smaller stepsize. This approach, while effective, can be inefficient and probably cannot be implemented for real-time problems, where a globally accurate result is needed before the next iteration. It is not our intention to report on methods which address this issue, but we would like to take the opportunity to refer to our own recent work in this regard, where we have developed an algorithm based on high-order quenching to enable stepwise global error control [3][4].
5 Numerical example

An instructive example is the initial-value problem

\[
y' = \left( \frac{\ln 1000}{100} \right) y \\
y(0) = 1
\]

on \([0, 100]\). The coefficient in the differential equation has been chosen so that \(y\) does not exceed 1000 on \([0, 100]\), i.e. \(y\) does not vary substantially, so that absolute error control is suitable. The exact solution is \(y(x) = e^{\ln 1000 x}\).

We use RK3 [5] and RK4 [6] to implement local error control, with \(\delta = 10^{-8}\). The quantities \(|\varepsilon^3|\) and \(|\alpha^3,4 \Delta^4|\) are shown as functions of \(x\) in Figure 1 (figure follows appendix). We see that the local error \(|\varepsilon^3|\) is bounded by \(\delta\), as expected. However, \(|\alpha^3,4 \Delta^4|\) increases monotonically. The global error \(|\Delta^3,4|\) is given by \(|\varepsilon^3 + \alpha^3,4 \Delta^4|\) and, although not shown, it is easy to see that \(|\Delta^3,4|\) must increase beyond \(\delta\), and is almost 100 times greater than \(\delta\) at \(x = 100\). In fact, \(|\Delta^3,4|\) becomes larger than \(\delta\) at \(x = 23.6\), after 118 iterations. This is the value of \(i\) for which (11) is violated for this example. For \(x < 23.6\), the condition is not violated and the global error is bounded by \(\delta\). Clearly, though, this state of affairs does not last, and the propagation of \(\Delta^4\) eventually compromises the global accuracy of the solution.

6 Conclusion

We have investigated the relationship between local error and global error in RK methods, under the implementation of local error control via local extrapolation. We find that, even though local error is successfully controlled, we cannot expect the same for global error. Our analysis shows that there is a possibility that the global error will be bounded by a user-imposed tolerance during the initial stage of the integration, but this will not last. The propagation of the global error in the higher-order method will eventually cause the global error in the lower-order method to exceed the tolerance. A numerical example clearly illustrates these points.

References

[1] Hairer, E., Norsett, S.P., and Wanner, G. (2000). Solving Ordinary Differential Equations I: Nonstiff Problems, Berlin: Springer.

[2] Prentice, J.S.C. (2009). General error propagation in the RKRGLm method, Journal of Computational and Applied Mathematics, 228, 344-354.

[3] Prentice, J.S.C. (2011). Stepwise global error control in an explicit Runge-Kutta method using local extrapolation with high-order se-
lective quenching, *Journal of Mathematics Research*, 3, 2, 126-136. [http://ccsenet.org/journal/index.php/jmr/article/view/8700/7481]

[4] Prentice, J.S.C. (2011). Relative global error control in the RKQ method for systems of ordinary differential equations, *Journal of Mathematics Research*, 3, 4, 59-66. [http://ccsenet.org/journal/index.php/jmr/article/view/10491/8952]

[5] Kincaid, D., and Cheney, W. (2002). *Numerical Analysis: Mathematics of Scientific Computing 3rd ed.*, Pacific Grove: Brooks/Cole.

[6] LeVeque, R.J. (2007). *Finite Difference Methods for Ordinary and Partial Differential Equations*, Philadelphia: SIAM.

7 Appendix

7.1 The assumption $|\beta_{i+1}^z (x_i - x_0) h^{z+1} + 1| < \delta$

Assuming a constant stepsize $h$, the underlying premise of local extrapolation is the assumption that

$$|\beta_{i+1}^z h^{z+1}| > |\beta_{i+1}^{z+1} h^{z+2}|,$$

which implies

$$|\beta_{i+1}^z h^{z+1}| = M |\beta_{i+1}^{z+1} h^{z+2}|,$$

where $M \gg 1$ is a large number. Assuming that $\beta_{i+1}^{z+1}$ is a slowly varying function of $x$, we can replace $\beta_{i+1}^{z+1}$ with its average value $\bar{\beta}_{i+1}^{z+1}$, and so we may write

$$|\beta_{i+1}^z h^{z+1}| > i |\bar{\beta}_{i+1}^{z+1} h^{z+2} = |\bar{\beta}_{i+1}^{z+1} (x_i - x_0) h^{z+1}|,$$

subject to the condition that $i < M$. Hence,

$$|\beta_{i+1}^z h^{z+1} < \delta \Rightarrow |\bar{\beta}_{i+1}^{z+1} (x_i - x_0) h^{z+1} < \delta.$$
Figure 1: Error components $|\varepsilon^3|$ and $|\alpha^{3,4}\Delta^4|$ for the example. Global error $|\Delta^{3,4}|$ (not shown) is the sum of these two components.