In search of stability: Runge–Kutta methods and Richardson extrapolation

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I. Overview

In the previous semester we reviewed several generalization of A-stability, namely AN-, B/BN- and algebraic-stability [1]. We then went on and stated how these stability types relate to each other, which we shall state again, since we will use these relations in this work.

Theorem. *For a nonconfluent RK method the following implications hold:*

$$\left\{\begin{array}{c}\textit{Algebraic stability}\\ \Updownarrow \\ \textit{BN-stability}\\ \Updownarrow \\ \textit{AN-stability}\end{array}\right\} \Longrightarrow \textit{B-stability} \Longrightarrow \textit{A-stability}.$$

For a general RK method the following implications hold:

$$\textit{Algebraic stability} \Longrightarrow \left\{\begin{array}{ccc}\textit{BN-stability} & \Rightarrow & \textit{B-stability}\\ & & \Downarrow \\ \textit{AN-stability} & \Rightarrow & \textit{A-stability}\end{array}\right\}.$$

In our previous work we did not go into detail how hard it is to find methods which possess any of the above stability properties. In this work one of our goals is to present some parameterized methods and give conditions on the stability properties of these methods.

While our primary focus is stability, we will impose order conditions: specifically an s-stage Runge–Kutta method should achieve order s, or at the very least order $s-1$.

II. 2-stage methods

We focused on diagonally implicit Runge–Kutta methods (DIRKs), as the reduced number of variables helped simplify computations. A general 2-stage nonconfluent ($a_1 \neq a_2 + a_3$) DIRK method with first order consistency has the following Butcher tableau:

$$\begin{array}{c|cc} a_1 & a_1 & 0 \\ a_2 + a_3 & a_2 & a_3 \\ \hline & b & 1-b \end{array}$$

Table 1: 2-stage nonconfluent DIRK methods' Butcher tableau

Since the method is nonconfluent, we only need to check the conditions for algebraic stability. With this in mind, the matrices B and M are the following:

$$B = \begin{pmatrix} b & 0 \\ 0 & 1-b \end{pmatrix}$$

$$M = \begin{pmatrix} 2a_1 b - b^2 & (1-b)a_2 - b(1-b) \\ (1-b)a_2 - b(1-b) & 2a_3(1-b) - (1-b)^2 \end{pmatrix}$$

We require positive semidefiniteness, for the matrix B this will hold if $b \in [0,1]$. To compute the condition for M we will impose the following simplifications: $a_1 = a_3 := a$, i.e., the diagonal values are the same, and $b = 1/2$. In view of this M modifies into

$$M = \begin{pmatrix} a - \frac{1}{4} & \frac{1}{2}a_2 - \frac{1}{4} \\ \frac{1}{2}a_2 - \frac{1}{4} & a - \frac{1}{4} \end{pmatrix}.$$

The quadratic form will be

$$\underline{x}^\intercal M \underline{x} = \left(a - \frac{1}{4}\right)x^2 + \left(a_2 - \frac{1}{2}\right)xy + \left(a - \frac{1}{4}\right)y^2$$

By completing the square and introducing second order condition we get the following conditions:

$$\begin{aligned} 2a &= a_2 \\ 1 &= 2a + a_2 \end{aligned}$$

Thus,

$$a = \frac{1}{4}, \qquad a_2 = \frac{1}{2}$$

and our Butcher tableau will take the following form:

$$\begin{array}{c|cc} \frac{1}{4} & \frac{1}{4} & 0 \\ \frac{3}{4} & \frac{1}{2} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Table 2: 2-stage second order algebraically stable DIRK method

The method corresponding to this Butcher tableau is called Qin and Zhang's method, which has good stability properties and in bonus is a symplectic integrator.

One can see that this approach is rather tedious and was only successful after introducing new simplifying conditions. Moreover, only a single method was derived. To obtain more general results, we will begin by stating the order conditions and then proceed towards a stability analysis.

Our general methods will take the form provided by Pareschi and Russo [2]:

a	a	0
$1-a$	$1-2a$	a
	$\frac{1}{2}$	$\frac{1}{2}$

Table 3: 2-stage second order general DIRK method

One can verify with the order conditions that this setup will result in a second order method.

$$\sum b_i = 1 \iff \frac{1}{2} + \frac{1}{2} = 1$$
$$\sum b_i c_i = \frac{1}{2} \iff \frac{1}{2}a + \frac{1}{2}(1-a) = \frac{1}{2}$$

For third order both conditions $\sum b_i c_i^2 = \frac{1}{3}$ and $\sum\sum b_i a_{ij} c_j = \frac{1}{6}$ must be satisfied. Both of these conditions are met if $a^2 - a + \frac{1}{6} = 0$ holds. Hence the method will be third order with the roots $a = \frac{3\pm\sqrt{3}}{6}$.

With $b_1 = b_2 = 1/2$ the $B = \frac{1}{2}I$ matrix will be positive semidefinite. The matrix M will take the following form:

$$M = \begin{pmatrix} a - \frac{1}{4} & \frac{1}{4} - a \\ \frac{1}{4} - a & a - \frac{1}{4} \end{pmatrix}.$$

From this the eigenvalues are $\lambda_1 = 0$ and $\lambda_2 = 2(a - \frac{1}{4})$. Therefore the condition for algebraic stability will be $a \geq \frac{1}{4}$. If we take third order into account, only the method with $a = \frac{3+\sqrt{3}}{6}$ will possess algebraic stability.

One more question still remains: Is the condition $a \geq \frac{1}{4}$ the requirement for A-stability too for these methods? To answer this we have to check the condition for the stability function that has the form

$$R_a(z) = \frac{1 + (1-2a)z + \left(a^2 - 2a + \frac{1}{2}\right) z^2}{(1-az)^2}.$$

To check the condition for A-stability we will use the following theorem [3].

Theorem. *Let the stability function $R(z)$ be of the form $R(z) = \frac{N(z)}{D(z)}$ where N and D is a polynomial of z and define the E-polynomial by*

$$E(y) = D(iy)D(-iy) - N(iy)N(-iy).$$

A Runge–Kutta method with stability function $R(z)$ is A-stable if and only if all poles of R (that is all roots of D) are in the right half plane, and $E(y) \geq 0 \ \forall y \in \mathbb{R}$.

The root of $D(z)$ is $z = \frac{1}{a}$, $a \neq 0$ and it is in the right half plane when $a > 0$. After some algebraic manipulation the method's E-polynomial can be expressed as

$$E(y) = \left(a^4 - \left(a^2 - 2a + \frac{1}{2}\right)^2\right) y^4.$$

Equivalently,

$$E(y) = \frac{1}{4}(1-2a)^2(4a-1)y^4.$$

Thus the second condition in the theorem is satisfied when

$$a \geq \frac{1}{4}.$$

In conclusion we found that $a \geq \frac{1}{4}$ is the condition for A-stability too. From this it follows that the third order method, with $a = \frac{3-\sqrt{3}}{6}$ does not have good stability properties.

The next method we investigated is defined by the Butcher tableau:

a	a	0
1	$1-a$	a
	$1-a$	a

Table 4: 2-stage first order general DIRK method

Clearly, this method has at least first order, and it has second order if a is root of $a^2 - 2a + \frac{1}{2} = 0$, namely when $a = \frac{2\pm\sqrt{2}}{2}$. For finding the conditions for algebraic stability, we go through the same steps as before. For the matrix $B = \begin{pmatrix} 1-a & 0 \\ 0 & a \end{pmatrix}$ to be positive semidefinite the condition $a \in [0,1]$ must hold. The matrix M will take the diagonal form

$$M = \begin{pmatrix} -3a^2 + 4a - 1 & 0 \\ 0 & a^2 \end{pmatrix}.$$

The second eigenvalue $\lambda_2 = a^2$ will be non-negative for any a, and the first eigenvalue $\lambda_1 = -3a^2 + 4a - 1$ is non-negative if $a \in \left[\frac{1}{3}, 1\right]$. Therefore, the method will be algebraically stable when a is in the interval $\left[\frac{1}{3}, 1\right]$. Since the values $a = \frac{2\pm\sqrt{2}}{2}$ are not in this interval, we only found first order algebraically stable methods.

To check if the second order methods are A-stable, we first derive the stability function and then apply the previous theorem. The R function will take the form

$$R_a(z) = \frac{1 + (1-2a)z}{(1-az)^2}.$$

The root of $D(z)$ is the same as before, therefore $a > 0$ must hold. The $E(y)$ polynomial is

$$E(y) = a^4 y^4 - (2a^2 - 4a + 1)y^2.$$

The condition $E(y) \geq 0$ is satisfied when

$$\frac{2-\sqrt{2}}{2} \leq a \leq \frac{2+\sqrt{2}}{2}.$$

In conclusion we managed to extend the set of stable methods and we showed that the second order methods will be A-stable.

Our next method is given by Crouzeix [4, 5] and it is defined by the following Buthcer tableau:

$$
\begin{array}{c|cc}
\frac{3\mu-1}{6\mu} & \frac{3\mu-1}{6\mu} & 0 \\
\frac{1+\mu}{2} & \mu & \frac{1-\mu}{2} \\
\hline
 & \frac{3\mu^2}{3\mu^2+1} & \frac{1}{3\mu^2+1}
\end{array}
$$

Table 5: 2-stage third order general DIRK method

One can verify by checking all four order conditions that this method has third order for all $\mu \neq 0$. We now turn to the study of algebraic stability. Since both values b_i are strictly positive, the matrix B is positive semidefinite. Checking this condition for matrix M will take a bit more finesse. Due to the expression $3\mu^2+1$ in the denominators of b_i and the $bb^\intercal$ part in the definition of M we have rational functions of μ in the elements of the matrix. By factoring the denominator, M takes the following form:

$$M = \frac{1}{(3\mu^2+1)^2}\widetilde{M}$$

$$\widetilde{M} = \begin{pmatrix} (3\mu^2-\mu)(3\mu^2+1)-9\mu^2 & \mu(3\mu^2+1)-3\mu^2 \\ \mu(3\mu^2+1)-3\mu^2 & (1-\mu)(3\mu^2+1)-1 \end{pmatrix}.$$

By simplifying $\widetilde{M}$, the expression $\mu(3\mu^2-3\mu+1)$ appears in all of the elements. After factoring it out $\widetilde{M}$ becomes

$$\widetilde{M} = \mu(3\mu^2-3\mu+1)\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$$

Thus M can be written in its final form as

$$M = \frac{\mu(3\mu^2-3\mu+1)}{(3\mu^2+1)^2}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Since the eigenvalues of $\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$ are $\lambda_1 = 0$ and $\lambda_2 = -2$, M can only be positive semidefinite if the coefficient is nonpositive. Since the denominator and the expression $3\mu^2-3\mu+1$ is always positive, the condition for algebraic stability will be $\mu < 0$.

A good choice for μ can be $\mu = -\frac{\sqrt{3}}{3}$. This method's Butcher tableau then becomes

$$
\begin{array}{c|cc}
\frac{3+\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} & 0 \\
\frac{3-\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

With this choice we get rational weights and our c_i values will be Gaussian interpolation points.

III. 3-stage methods

Our first and only 3-stage third order DIRK method will be provided by Crouzeix once again [5]. The corresponding Buthcer tableau is the following:

$$
\begin{array}{c|ccc}
\frac{1+v}{2} & \frac{1+v}{2} & 0 & 0 \\
\frac{1}{2} & -\frac{v}{2} & \frac{1+v}{2} & 0 \\
\frac{1-v}{2} & 1+v & -1-2v & \frac{1+v}{2} \\
\hline
 & \frac{1}{6v^2} & 1-\frac{1}{3v^2} & \frac{1}{6v^2}
\end{array}
$$

Table 6: 3-stage third order general DIRK method

For $v \neq 0$ the third order can be verified and we can achieve fourth order if v is the root of $3v^3-3v-1=0$. These roots are

$$v_1 = \frac{2}{\sqrt{3}}\cos\frac{\pi}{18}$$
$$v_2 = -\frac{2}{\sqrt{3}}\cos\frac{5\pi}{18}$$
$$v_3 = -\frac{2}{\sqrt{3}}\cos\frac{7\pi}{18}$$

The analysis of algebraic stability will be the same as before. For B to be positive semidefinite we demand that the values of b_i be non-negative, thus our first condition is $v^2 \geq \frac{\sqrt{3}}{3}$. When constructing the matrix M and calculating its eigenvalues, we run into the same tedious work as we did before but with a new twist this time. Factoring out the square of values $b_{1,3}$, M takes the form

$$M = \frac{1}{36v^4}\widetilde{M}$$

$$\widetilde{M} = \begin{pmatrix} 6v^3+6v^2-1 & -18v^5+6v^3-6v^2+2 & 6v^3+6v^2-1 \\ -18v^5+6v^3-6v^2+2 & 36v^5-12v^3+12v^2-4 & -12v^3-12v^2+2 \\ 6v^3+6v^2-1 & -12v^3-12v^2+2 & 6v^3+6v^2-1 \end{pmatrix}.$$

Here we use the fact that the method has fourth order when $3v^3-3v-1=0$. By applying this relation repeatedly we eliminate the higher order terms of $\widetilde{M}$ until only quadratic polynomials remain in the elements. After this process one can see that the term $6v^2+6v+1$ appears in all of the elements. Factoring it out M takes the form

$$M = \frac{6v^2+6v+1}{36v^4}\begin{pmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{pmatrix}.$$

The eigenvalues of this new matrix are $\lambda_{1,2} = 0$ and $\lambda_3 = 6$. Thus the condition for algebraic stability (when the method is fourth order) will be $6v^2+6v+1 \geq 0$. Out of the three roots, only $v_1 = \frac{2}{\sqrt{3}}\cos\frac{\pi}{18}$ satisfies this condition.

At this point the reader might ask about four-stage methods or fully implicit methods. In practice the literature rarely goes beyond three- and four-stages due to calculations getting increasingly complicated and tedious. Our choice of the DIRK methods was to maximize the number of zero elements, while giving meaningful insight into what conditions must be met for desirable stability properties.

IV. Richardson extrapolation

Richardson extrapolation [6] is a convergence acceleration method, and it is widely used for improving the order of convergence of iterative numerical methods. One can use it to improve numerical integration: by applying Richardson extrapolation to the trapezoid rule we get Romberg's method. Other applications include the numerical solutions of ODEs and PDEs, naturally our focus will be on Richardson extrapolation applied to Runge–Kutta methods.

Suppose that we have an ODE in the form of $y'(t) = f(t, y(t))$, which we intend to solve numerically. Suppose further that we have an equidistant grid with stepsize h, and a Runge–Kutta method of order p. (Note that the following method can be extended to multistep methods.) Then, our extrapolated method will be the following for calculating y_{n+1}:

- take a step with h: $v_{n+1} \approx y(t_{n+1})$,
- take two steps with $h/2$: $w_{n+1} \approx y(t_{n+1})$,
- calculate y_{n+1} using $y_{n+1} = \dfrac{2^p w_{n+1} - v_{n+1}}{2^p - 1}$.

One can show with the original method being of order p that $y(t_{n+1}) - \dfrac{2^p w_{n+1} - v_{n+1}}{2^p - 1} = \mathcal{O}(h^{p+1})$, thus the extrapolated method increases the order of accuracy by at least one.

Now that we designed a new method, we must answer the following question: In what situation should we choose the new method over the original? Let A denote our original numerical integrator, and let B denote our new method. When A is explicit and we apply both methods to the problem with the same stepzise h, method B will take 3 times more steps to calculate the next value. However, method B has higher order of accuracy, we are not required to use the same stepsize for both methods. If $h_B > 3h_A$, method B will be computationally more efficient.

When the underlying method A is implicit, the solution must be found by solving a system of equations. As a result, a simple inequality cannot be stated for the stepsizes of methods A and B. The reason for this lies in the application of different root finding methods.

There is one more question we should answer before applying Richardson extrapolations: Will the improved approximation of y_{n+1} take part in calculating the next approximations or not? By answering it with yes or no, we obtain two different applications of Richardson extrapolation. When the improved calculations do not take part in calculating the next step, we obtain the *passive* Richardson extrapolation, and when they do take part we obtain the *active* Richardson extrapolation. One can visualize the two implementations in the following way:

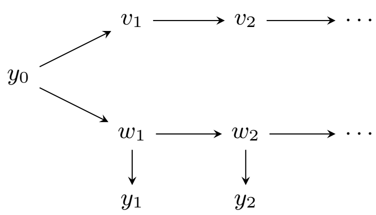

Figure 1: Passive implementation of Richardson extrapolation

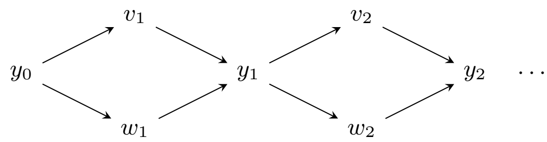

Figure 2: Active implementation of Richardson extrapolation

Passive implementation can be thought of in the following way: We take two equidistant grids with h and $h/2$, and we solve the problem with the original method on both grids. Then we calculate y_i from the values v_i and w_i. In the active implementation we only have one grid with stepsize h. During the iteration we use the previously calculated y_n values for calculating v_{n+1} and w_{n+1}. In our study we will only consider the active implementation.

V. Stability analysis of Richardson extrapolated methods

For applying Richardson extrapolation to RK methods we will state the following goal: The new method should achieve the same stability properties as the underlying method, or preferably, attain improved stability properties.

Once again suppose our RK method has order of p, with the stability function $R(z)$. To calculate the stability function of the extrapolated method, we apply our RK method to Dahlquist's test equation. The values v_{n+1} and w_{n+1} will be calculated in the following way:

$$v_{n+1} = R(z) y_n,$$
$$w_{n+1} = R^2\left(\frac{z}{2}\right) y_n.$$

Thus,

$$y_{n+1} = \frac{2^p w_{n+1} - z_{n+1}}{2^p - 1} y_n = \frac{2^p R^2\left(\frac{z}{2}\right) - R(z)}{2^p - 1} y_n.$$

Therefore the stability function of the Richardson extrapolated method will take the form:

$$R_{RE}(z) = \frac{2^p R^2\left(\frac{z}{2}\right) - R(z)}{2^p - 1}$$

We now turn to explicit methods. It is well known that the stability for explicit methods with same number of stages (s) and order (p) the stability function R is uniquely defined. For these methods we state the following statement.

Theorem. *For any Runge–Kutta method with $s = p$, $p = 1, 2, 3, 4$ orders and stages, the stability region of the Richardson extrapolated method is greater than the stability region of the underlying Runge–Kutta method.*

One can calculate the new R_{RE} functions and verify the statement. We only note an interesting fact: The function R_{RE} of the $s = p = 1$ explicit Euler method will be the same as the stability function of the second order explicit Runge–Kutta methods. We now show the increased stability regions for the methods stated in the previous theorem.

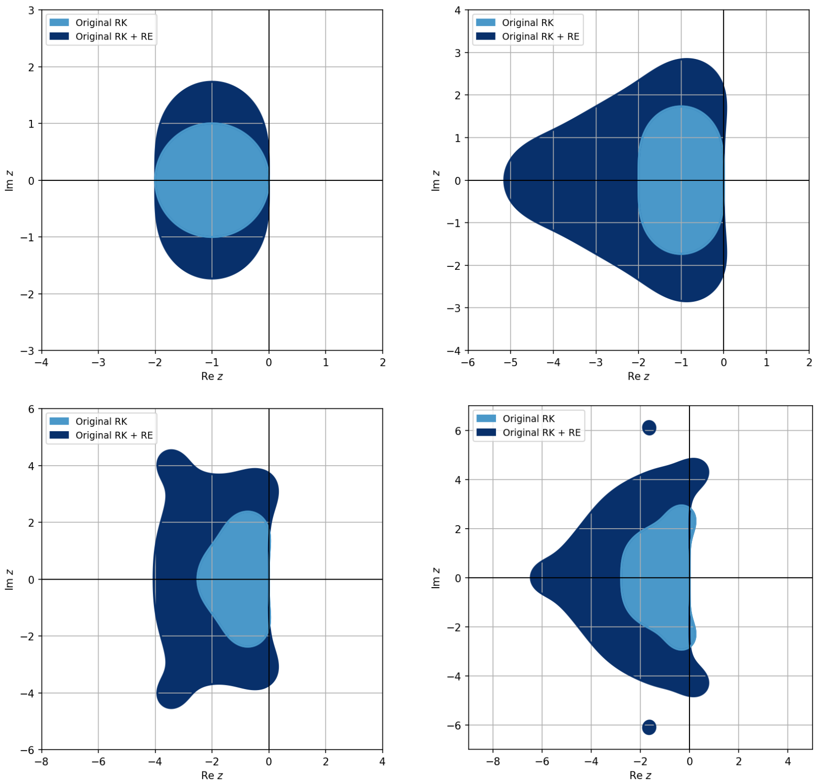

Figure 3: $s = p = 1, 2, 3, 4$ explicit Runge–Kutta and their Richardson extrapolated methods' stability regions

What if $s \neq p$? When the order is lower than the number of stages, the stability function of an explicit RK method takes the form:

$$R(z) = 1 + z + \ldots + \frac{z^p}{p!} + \frac{z^{p+1}}{\gamma_{p+1}^{(s,p)}(p+1)!} + \ldots + \frac{z^s}{\gamma_s^{(s,p)}s!}$$

In this expression we have $s - p$ free parameters to modify in order to get even larger stability regions for the underlying method and for the extrapolated method.

We will consider the case where the order is $p = 3$ and there are $s = 4$ stages. With one free parameter the search is very straightforward. We iterate $\gamma_4^{(3,4)}$ on the interval $[1, 5]$ with stepsize 0.01. We consider a stability region acceptable if it contains the interval $[-6, 0]$ of the real axis and the stability region should stretch up to $4i$ and down to $-4i$ along the imaginary axis. This numerical experiment shows that $\gamma_4^{(3,4)} \approx 2.4$ is a good candidate for a number of reasons. First, the stability region of the underlying method is greater than that of the 3-stage third order explicit methods. Second, as we required, the stability region has grown significantly due to the extrapolation. Lastly, the new method possesses a larger stability region than the Richardson extrapolated $s = p = 3$ explicit Runge–Kutta methods.

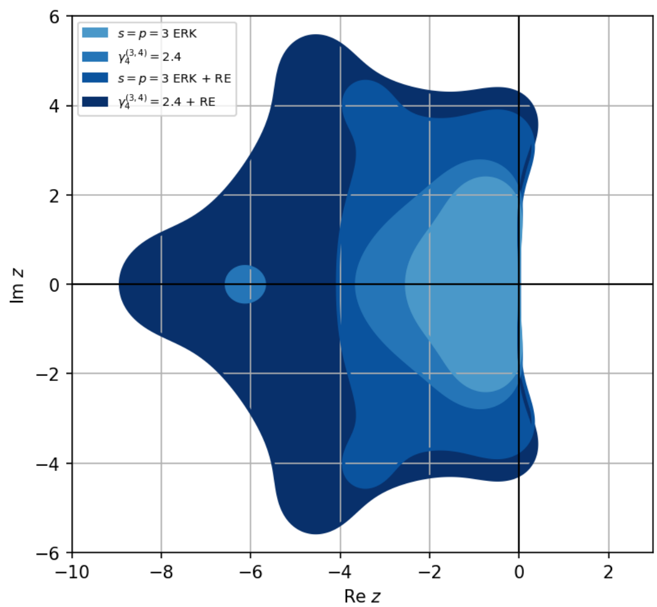

Figure 4: Stability function of $\gamma_4^{(3,4)} = 2.4$ compared with other stability regions

We conclude our study with the following conjecture.

Conjecture. *The application of Richardson extrapolation to any explicit Runge–Kutta method leads to a new numerical method which has a larger stability region.*

References

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