

On Spurious Fixed Points of Runge–Kutta Methods

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In this paper we investigate the onset of spurious fixed points when Runge–Kutta methods are applied to study the dynamics of differential equations. It is shown computationally that the spurious equilibria of Griffiths *et al.* [14] are connected at infinity with fixed points inherited from the differential equation. We introduce and study the concept of B-regularity which is in connection to the concept of regularity introduced by Iserles. © 1997 Academic Press

Principium cuius hinc nobis exordia sumet,
nullam rem e nilo gigni diuinitus umquam.
Nam si de nilo fierent, ex omnibus' rebus
omne genus nasci posset, nil semine egeret.
De rerum natura, Liber Primus, 149. Lucrecio

1. INTRODUCTION

The growing interest in dynamical systems, in particular in their chaotic behaviour, has stimulated a large amount of numerical investigation. Very often, numerical simulations are used to discover the dynamics of systems of differential equations.

From the point of view of numerical analysis, the following questions arise: Given a system of ordinary differential equations which is integrated by a given numerical method, is the dynamics of the approximate solution a faithful description of the dynamics of the continuous system? In particular, are all the invariant sets (fixed points, limit cycles, strange attractors) of the differential system approximated by the numerical method? Does the longtime behaviour of numerical trajectories simulate that of the continuous system?

The approximation of invariant sets has been studied by Braun and Hershenvov [3], Doan [7], Kloeden and Lorenz [24], Beyn [1, 2], Eirola [8, 9]. There are results that prove that, if the parameter h of the discretization is sufficiently small, the numerical method has an invariant set close and similar to that of the dynamical system. The question as to the longtime behaviour, for fixed step-size h and the number of steps becomes unbounded, is quite different. Brezzi, Ushiki, and Fujii [4] found spurious invariant cycles in Euler's method for a differential equation with a Hopf bifurcation. Griffiths and Mitchell [13], Sleeman *et al.* [28], Mitchell and Schoombie [26], Schoombie

[27], and Stuart [29] found spurious periodic solutions in convergent methods for nonlinear reaction–diffusion equation. Iserles [20] showed the existence of spurious fixed points in Runge–Kutta methods and predictor–corrector methods.

In this paper we shall consider Runge–Kutta methods applied to the autonomous scalar initial-value problem

$$\begin{aligned} u' &= f(u), \quad t \geq t_0, \\ u(t_0) &= u_0. \end{aligned} \quad (1.1)$$

This problem has a *fixed point* u^* , also known as equilibrium point, critical point, or steady-state solution, when

$$f(u^*) = 0. \quad (1.2)$$

If $f'(u^*) < 0$, the fixed point is stable (neighbouring solutions are attracted to it), if $f'(u^*) > 0$ is unstable (neighbouring solutions are repelled). The case $f'(u^*) = 0$ is degenerate and the stability of u^* cannot be established by linearizing the differential equation.

A Runge–Kutta method may be written in the form

$$u_{n+1} = u_n + h \cdot \phi(u_n, h), \quad (1.3)$$

where ϕ is the increment function of the method. The numerical fixed points are the values u_h^* such that $u_n = u_h^*$ for each n and consequently satisfy

$$\phi(u_h^*, h) = 0. \quad (1.4)$$

Its stability or instability depends on whether $|1 + h(\partial\phi/\partial u)(u_h^*, h)| < 1$ or > 1 .

Let F be the set of all zeros of f , and let F_h denote the set all zeros of ϕ . Iserles [20] has proved that $F \subset F_h$, but $F_h \setminus F$ may be nonempty, so that the Runge–Kutta method may have *spurious fixed points*, steady solutions which are a result of the discretization and not a feature of the underlying differential equation and may, consequently, lead to erroneous computational results. As we shall show later, these spurious fixed points may appear below the

linearized stability limit of the scheme. Stable spurious fixed points are undesirable since they attract a subset of the initial states and this asymptotic behaviour of the scheme is clearly incorrect (Mitchell and Griffiths [13], Iserles [20]). Unstable manifolds of spurious solutions are often connected to infinity (Mitchell and Griffiths [13], Stuart [29], Humphries [19]) and may affect the basin of attraction of the *essential fixed points*, that is, the fixed points of the differential equation.

The aim of this paper is to study why there exist these spurious equilibria. The numerical method is considered as a dynamical system parameterized by the time-step h and we apply techniques from bifurcation theory (Chow and Hale [5]) and singularity theory (Golubisky and Schaeffer [12]). We show that spurious fixed points bifurcate from essential steady solutions of the numerical methods (Stuart [29], Iserles, Peplow, and Stuart [21]). If we know the origin of the spurious solutions we can prevent their appearance and we may find Runge–Kutta methods that $F_h \equiv F$; i.e., methods that are regular in the sense of Iserles [20].

In Section 2 we study the branches of spurious fixed points of some explicit Runge–Kutta schemes applied to the logistic equation (Griffiths *et al.* [14]). We show computationally that all spurious fixed points bifurcate from true fixed points. In Section 3 we consider implicit Runge–Kutta methods and study conditions in order to avoid possible bifurcation of essential fixed points. In Section 4 we consider the bifurcation of real fixed points and make some final comments.

2. BRANCHES OF SPURIOUS FIXED POINTS FOR EXPLICIT RUNGE–KUTTA METHODS

Griffiths, Sweby, and Yee [14] have investigated analytically and computationally explicit Runge–Kutta schemes applied to the equation

$$u' = f(u) = u(1 - u), \tag{2.1}$$

with two equilibrium points $u = 1$, stable, and $u = 0$, unstable. In particular, they consider five explicit Runge–Kutta methods (Lambert [23]):

- (i) Explicit Euler.
- (ii) Modified Euler.
- (iii) Improved Euler.
- (iv) Heun, a 3-stage third-order method.
- (v) The classical 4-stage fourth-order Runge–Kutta method.

Some fixed points may be determined with the help of an algebraic manipulation package: MAPLE, DERIVE, or MATHEMATICA. Other equilibria have been found

TABLE I

Scheme	Fixed points	Stable range
Explicit Euler	1	$0 < h < 2$
Modified Euler	1	$0 < h < 2$
	$1 + \frac{2}{h}$	$0 < h < -1 + \sqrt{5} \approx 1.236$
	$\frac{2}{h}$	$2 < h < 1 + \sqrt{5} \approx 3.236$
Improved Euler	1	$0 < h < 2$
	$\frac{2 + h \pm \sqrt{h^2 - 4}}{2h}$	$2 < h < \sqrt{8} \approx 2.828$
Heun	1	$0 < h < 2.513$
	*	$4.9137 < h < 4.9552$
	*	$6.4799 < h < 6.4853$
	*	$6.74405 < h < 6.74575$
RK4	1	$0 < h < 2.785$
	*	$2.785 < h < 3.4156$
	*	$2.746 < h < 3.456$

Note. The entries with an asterisk mean that fixed points are known to exist but no closed analytic form has been found.

computationally. The results are listed in Table I with the corresponding stability range.

The family of explicit Runge–Kutta methods of two stages and order 2 can be written in Butcher’s notation as

$$\begin{array}{c|cc}
 0 & 0 & 0 \\
 \frac{1}{2b} & \frac{1}{2b} & 0 \\
 \hline
 & 1 - b & b
 \end{array} \tag{2.2}$$

I.e., the increment function is

$$\phi(u, h, b) = (1 - b)f(u) + bf\left(u + \frac{h}{2b} f(u)\right). \tag{2.3}$$

For $b = 1$ we recover the modified Euler method and for $b = \frac{1}{2}$, the improved Euler method.

Let u^* be a nondegenerate ($f'(u^*) \neq 0$) fixed point of (1.1). Then

$$\frac{\partial \phi}{\partial u}(u^*, h, b) = f'(u^*) \left((1 - b) + b \left(1 + \frac{h}{2b} f'(u^*) \right) \right) \tag{2.4}$$

and there exists a bifurcation point at

$$h^* = -\frac{2}{f'(u^*)}. \tag{2.5}$$

To identify the nature of the bifurcation we can use singularity theory (Golubnisky and Schaeffer [12]). Since

$$\frac{\partial^2 \phi}{\partial u^2}(u^*, h^*, b) = f''(u^*) \left(\frac{1}{b} - 2 \right), \quad (2.6)$$

and

$$\frac{\partial \phi}{\partial h}(u^*, h^*, b) = \frac{1}{2} f'(u^*) f(u^*) = 0, \quad (2.7)$$

$$\frac{\partial^2 \phi}{\partial u \partial h}(u^*, h^*, b) = \frac{1}{2} (f'(u^*))^2 > 0, \quad (2.8)$$

for $b \neq \frac{1}{2}$ we have a simple bifurcation or transcritical bifurcation; that is, the bifurcation is locally equivalent to the bifurcation in the origin of $\varepsilon v^2 + \lambda v$, where $\varepsilon = \text{sgn}((\partial^2 \phi / \partial u^2)(u^*, h^*, b))$. In particular for (2.1) $f''(u) = -2 < 0$ and then, if $b > \frac{1}{2}$ (for example, in the modified Euler method) $\varepsilon = 1$ and the normal form is $v^2 + \lambda v$ which corresponds exactly to Fig. 1, obtained with the help of the continuation software package AUTO and agrees with the results of Griffiths *et al.* (Table I). The labeling of the branches of the bifurcation diagram indicate the sign of $\partial \phi / \partial u$. The u corresponds to unstable fixed points, and s is negative to stable fixed points. However, in the stable branches first (for h corresponds to the right boundary of the stable range in Table I) $h(\partial \phi / \partial u) = -2$ and, then, there exists period-doubling bifurcation (Wiggins [32],

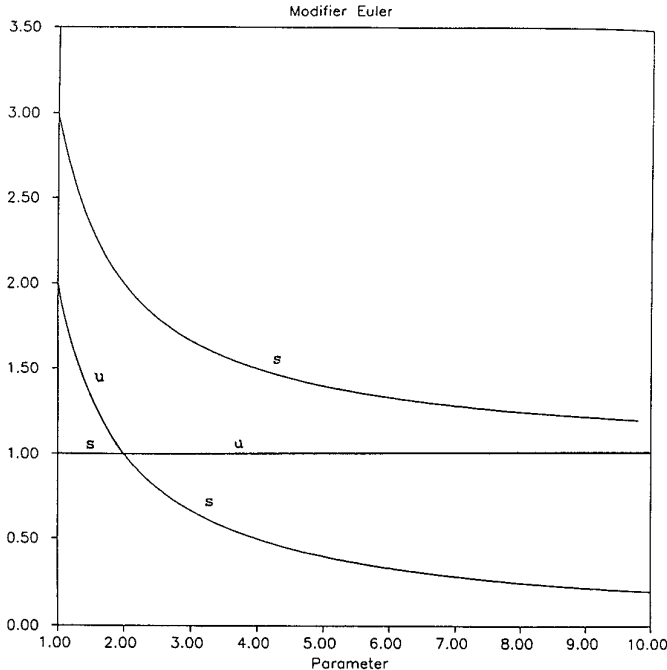


FIGURE 1

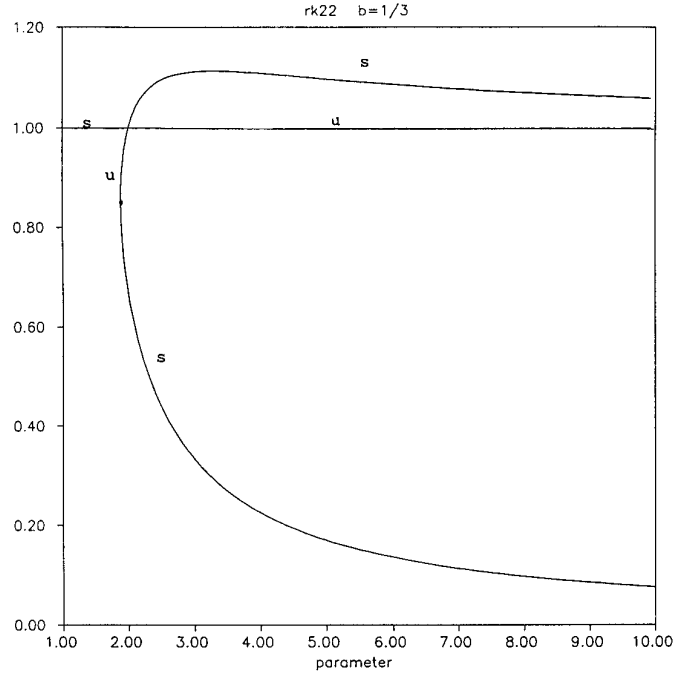


FIGURE 2

Thompson and Stewart [31], Guckenheimer and Holmes [15]) and the beginning the cascade in Fig. 2 of Griffiths *et al.* [14].

The branch of spurious fixed points $1 + 2/h$ appears below the linearized stability limit 2 and is not connected to any finite bifurcation point.

If $b < \frac{1}{2}$, $\varepsilon = -1$, for example, $b = \frac{1}{3}$; the normal form is $-v^2 + \lambda v$ which corresponds to Fig. 2, where the stable spurious fixed points with $h > 2$ are above $u = 1$.

Another type of bifurcation appears for the improved Euler method ($b = \frac{1}{2}$). Now $\partial^2 \phi / \partial u^2 = 0$ and

$$\frac{\partial^3 \phi}{\partial u^3} \left(u^*, h^*, \frac{1}{2} \right) = -f'''(u^*) + 3 \frac{(f''(u^*))^2}{f'(u^*)} \quad (2.9)$$

for (2.1) and $u^* = 1$, $f'''(1) = 0$, $f''(1) = -2$, $f'(1) = -1$, and

$$\frac{\partial^3 \phi}{\partial u^3} \left(1, 2, \frac{1}{2} \right) = -12 < 0. \quad (2.10)$$

The bifurcation is locally equivalent to $-v^3 + \lambda v$ and we have the pitchfork of Fig. 3. In this example, the spurious fixed points are out the stable range. A different nonlinear problem may be chosen to obtain spurious fixed points which turn back and exist for values $h < h^*$. By using again singularity theory, if $\partial^3 \phi / \partial u^3 > 0$ we would have a pitchfork, but open from right to left. For the polynomial

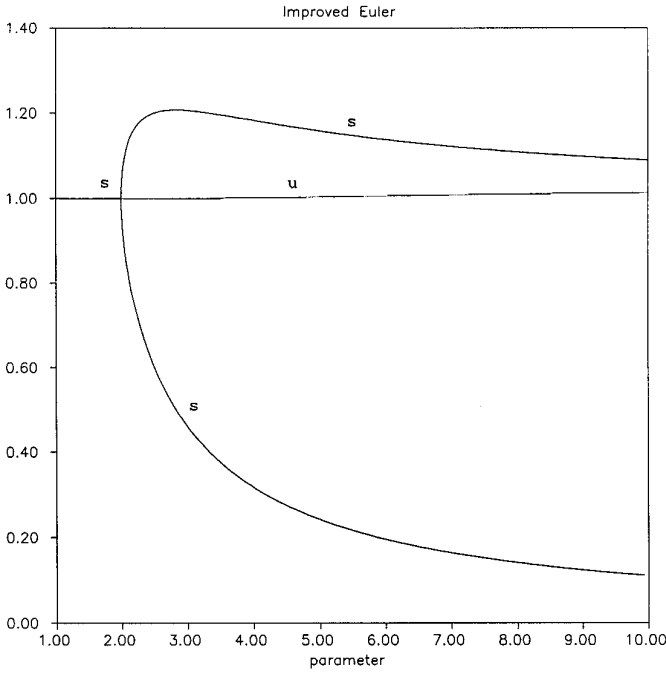


FIGURE 3

$$f(u) = -u^3 + 3u^2 - 4u + 2, \quad (2.11)$$

we have Fig. 4.

The analysis of Griffiths *et al.* [14] using perturbation arguments and the analysis above show that it is possible to predict the onset of spurious equilibria from essential fixed points and also to determine the nature of some bifurcations and the stability along the bifurcation branches. However, we do not yet understand the origin of some spurious fixed points, for example the branch $1 + 2/h$ in the modifier Euler method (Fig. 1 and Table I).

The Heun method applied to (2.1) has an increment function,

$$\begin{aligned} \phi(u, h) = & -\frac{4h^6}{243}u^4(u-1)^4 + \frac{16h^5}{81}u^3(u-1)^3\left(u - \frac{1}{2}\right) \\ & - \frac{8}{9}h^4u^2(u-1)^2\left(u^2 - u + \frac{1}{6}\right) \\ & + \frac{20}{9}h^3u^2(u-1)^2\left(u - \frac{1}{2}\right) \\ & - 4h^2u(u-1)\left(u^2 - u + \frac{1}{6}\right) \\ & + 4hu(u-1)\left(u - \frac{1}{2}\right) - 4u(u-1) \end{aligned} \quad (2.12)$$

and

$$\frac{\partial \phi}{\partial u}(0, h) = \frac{2}{3}h^2 + 2h + 4 > 0, \quad h \geq 0 \quad (2.13)$$

$$\frac{\partial \phi}{\partial u}(1, h) = -\frac{2}{3}h^2 + 2h - 4 < 0, \quad h \geq 0 \quad (2.14)$$

and there are not any finite bifurcation points. However, for large h (2.12) is similar to $u^4(u-1)^4$ and each fixed point for (2.12) generates a fixed point of multiplicity four. In other words, from a bifurcation at infinity the branches of spurious fixed points come from the right to the left as h decreases. These branches correspond to the asterisks in Table I. With the help again of the continuation software package AUTO we have obtained Fig. 5, where we have plotted the branches of fixed points of (2.12) which confirm the comments before. The left boundary of stable ranges in Table I corresponds exactly to the limit points of the branch in Fig. 5.

For the classical 4-stage Runge–Kutta(v) applied to (2.1)

$$\phi(u, h) = -\frac{h^{16}}{4096}u^8(u-1)^8 + \dots \quad (2.15)$$

Then for large h each of the fixed point generates a fixed point of multiplicity eight, so there should exist more branches of spurious equilibria than those reported by Griffiths *et al.* in their Table I. In fact, in Fig. 6 we plot a

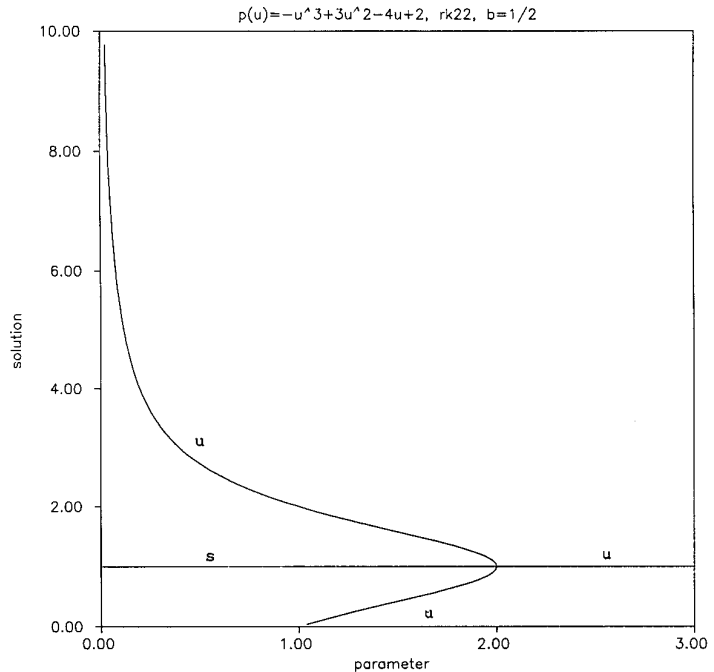


FIGURE 4

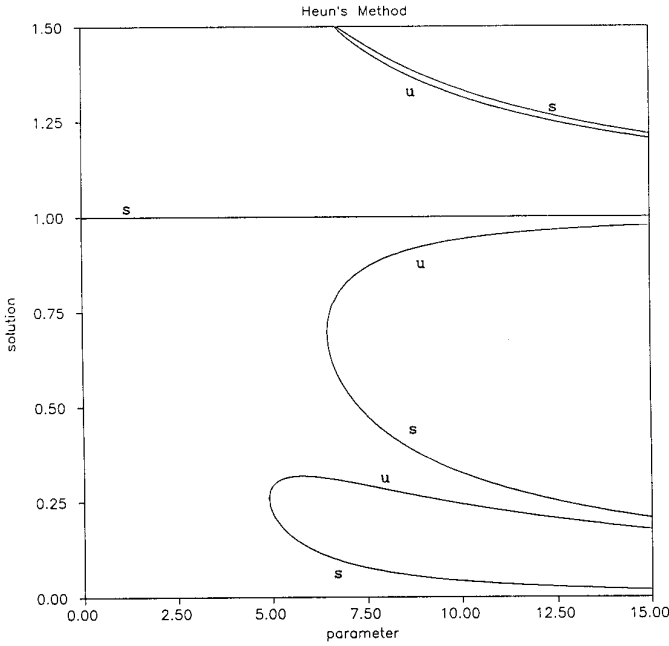


FIGURE 5

new branch of fixed points of (2.15), that is quite close to the unstable solution $u = 0$.

In general, for every explicit Runge–Kutta method with s stages if $f(u)$ is a polynomial of degree m , then $\phi(u, h)$ is polynomial of degree m^s . Then, for large h , each of the fixed points of $f(u)$ generates a fixed point of multiplicity

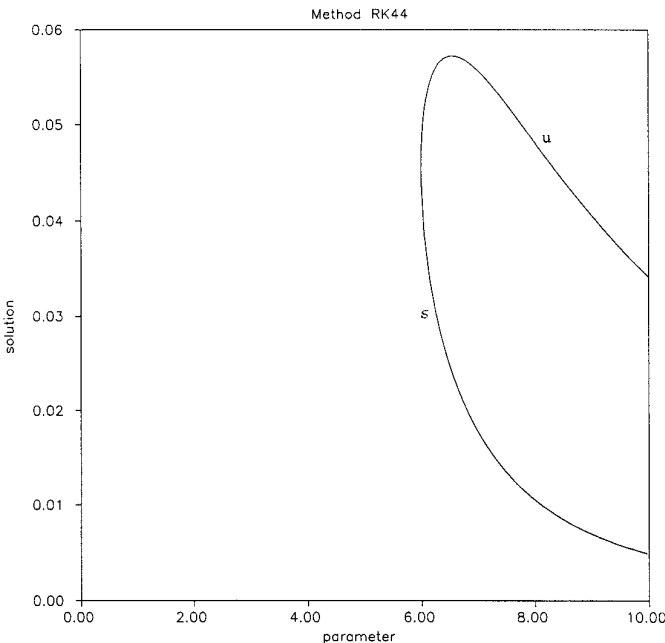


FIGURE 6

m^{s-1} and $m^{s-1} - 1$ of these are spurious and they are in branches of equilibria from bifurcation at infinity. To sum up every explicit Runge–Kutta method with $s > 1$ is irregular and has spurious fixed points that bifurcate at infinity from essential fixed points.

3. REGULARITY AND B-REGULARITY OF RUNGE–KUTTA METHODS

We consider a general s -stage method written as

$$\xi_i = f(u_n + h \sum_{j=1}^s a_{i,j} \xi_j), \quad i = 1, \dots, s, \quad (3.1)$$

$$u_{n+1} = u_n + h \sum_{i=1}^s b_i \xi_i. \quad (3.2)$$

We denote the method (3.1)–(3.2) in the customary way as

$$\begin{array}{c|ccc} & c_1 & \dots & c_s \\ \mathbf{c} & a & \vdots & \mathbf{c}_s \\ \hline & \mathbf{b}^T & \mathbf{c}_s & \mathbf{c}_s \\ \hline & & b_1 & \dots & b_s \end{array} \equiv \begin{array}{ccc} a_{1,1} & \dots & a_{1,s} \\ \vdots & \ddots & \vdots \\ a_{s,1} & \dots & a_{s,s} \end{array} \quad (3.3)$$

where $c_i = \sum_{j=1}^s a_{i,j}$, A denotes the matrix entries $a_{i,j}$, and \mathbf{b} is the vector $(b_1, \dots, b_s)^T$. The increment function is

$$\phi(u, h) = h \sum_{i=1}^s b_i \xi_i(u, h), \quad (3.4)$$

where $\xi_i(u, h)$ is the solution of the implicit system

$$\xi_i = f(u + h \sum_{j=1}^s a_{i,j} \xi_j) \quad i = 1, \dots, s. \quad (3.5)$$

Let F be the set of all zeros of f , and let F_h denote the set all zeros of ϕ which depend on h . In line with Iserles [20] we say that a method (3.3) is *regular*, if $F = F_h$ for all $h > 0$ and all initial value problems (remember that $F \subset F_h$ for all Runge–Kutta methods). Iserles proved the following theorem.

THEOREM 3.1. *A two-stage Runge–Kutta method of order $p \geq 2$ is regular if and only if $a_{1,1} + a_{2,2} = \frac{1}{2}$.*

From Section 2 it is clear that a necessary condition for a Runge–Kutta method to be regular is that each fixed point u^* of the differential equation does not bifurcate. This bifurcation is possible whenever $(\partial\phi/\partial u)(u^*, h) = 0$. Differentiating (3.4) and (3.5),

$$\frac{\partial \phi}{\partial u}(u^*, h) = h \sum_{i=1}^s b_i \frac{\partial \xi_i}{\partial u}(u^*, h) \quad (3.6)$$

$$\frac{\partial \xi_i}{\partial u}(u^*, h) = f'(u^*) \left(1 + h \sum_{j=1}^s a_{i,j} \frac{\partial \xi_j}{\partial u} \frac{\partial \xi_j}{\partial u}(u^*, h) \right), \quad i=1, \dots, s, \quad (3.7)$$

and (3.7) is equivalent to

$$(1 - hf'(u^*)a_{i,i}) \frac{\partial \xi_i}{\partial u}(u^*, h) = f'(u^*) + hf'(u^*) \quad (3.8)$$

$$\sum_{k \neq i} a_{i,j} \frac{\partial \xi_j}{\partial u}(u^*, h), \quad i = 1, \dots, s.$$

Let ξ denote the vector $(\xi_1, \dots, \xi_s)^\top$ and let $\mathbf{1}$ be the s -vector with unit entries $(1, \dots, 1)^\top$. Then (3.8) becomes

$$(I - hf'(u^*)A) \frac{\partial}{\partial u} \xi(u^*, h) = f'(u^*)\mathbf{1}. \quad (3.9)$$

In conclusion, the function (3.4) has a bifurcation point of the fixed point u^* if there exists a solution of the $[(s+1) \times s]$ -dimensional system,

$$(I - hf'(u^*)A) \frac{\partial}{\partial u} \xi(u^*, h) = f'(u^*)\mathbf{1}, \quad (3.10)$$

$$\mathbf{b}^\top \frac{\partial}{\partial u} \xi(u^*, h) = 0.$$

We are thus led to the $[(s+1) \times s]$ -dimensional linear system

$$(I - \lambda A) \cdot \eta(\lambda) = \mathbf{1}, \quad (3.11a)$$

$$\mathbf{b}^\top \cdot \eta(\lambda) = 0, \quad (3.11b)$$

where $\eta = (\eta_1, \dots, \eta_s)^\top$ and λ is a parameter. If we have a solution of (3.11) for some λ^* , there is a possible bifurcation point of u^* for the value of step h such that

$$h \cdot f'(u^*) = \lambda^*. \quad (3.12)$$

Since

$$B(\lambda) = \begin{pmatrix} I - \lambda A & \mathbf{1} \\ \mathbf{b}^\top & 0 \end{pmatrix} \quad (3.13)$$

is $(s+1) \times (s+1)$ and (3.11) is $[(s+1) \times s]$ -dimensional, then if $\det(B(\lambda)) \neq 0$ for each λ the system (3.11) has no solution, and u^* does not bifurcate.

EXAMPLE 3.2. A general nonconfluent ($c_1 \neq c_2$) Runge–Kutta method with two stages and second order can be written as

$$\begin{array}{c|cc} c_1 & a_{1,1} & c_1 - a_{1,1} \\ c_2 & c_2 - a_{2,2} & a_{2,2} \\ \hline & \frac{c_2 - 1/2}{c_2 - c_1} & \frac{1/2 - c_1}{c_2 - c_1} \end{array} \quad (3.14)$$

With the help of an algebraic manipulation package we obtain that

$$\det(B(\lambda)) = \lambda(a_{1,1} + a_{2,2} - \frac{1}{2}) - 1, \quad (3.15)$$

and $\det(B(\lambda)) \neq 0$ for each λ if and only if $a_{1,1} + a_{2,2} = \frac{1}{2}$ of Theorem 3.1 above.

To complete the proof, we consider the confluent case. Second order implies that $c_1 = c_2 = \frac{1}{2}$ and, using the algebraic manipulation package, we obtain again (3.15).

EXAMPLE 3.3. A general third-order SDIRK (simply diagonal implicit) method with three stages is given by

$$\begin{array}{c|ccc} \gamma & \gamma & & \\ c_2 & c_2 - \gamma & \gamma & \\ c_3 & c_3 - \alpha - \gamma & \alpha & \gamma \\ \hline & b_1 & b_2 & 1 - b_1 - b_2 \end{array} \quad (3.16)$$

with the conditions:

$$b_1 = \frac{3c_2(2c_3 - 1) - 3c_3 + 2}{6(c_2 - \gamma)(c_3 - \gamma)}, \quad (3.17)$$

$$b_2 = \frac{3c_3(2\gamma - 1) - 3\gamma + 2}{6(c_2 - c_3)(c_2 - \gamma)}, \quad (3.18)$$

$$\alpha = \frac{(-6\gamma^2 + 6\gamma - 1)(c_3 - \gamma)(c_2 - c_3)}{3c_2^2(2\gamma - 1) - 2c_2(3\gamma^2 - 1) + \gamma(3\gamma - 2)}. \quad (3.19)$$

Now

$$\det(B(\lambda)) = p_B(\lambda, \gamma) = -\frac{\lambda^2}{6}(3\gamma - 1)(6\gamma - 1) + \frac{\lambda}{2}(6\gamma - 1) - 1, \quad (3.20)$$

and for $\gamma = \frac{1}{6}$, a necessary condition for the regularity of (3.16) (Theorem 7 of Hairer, Iserles, and Sanz-Serna [17]), $p_B(\lambda, \frac{1}{6}) \equiv -1$.

For $\gamma = \frac{1}{3}$, $p_B(\lambda, \frac{1}{3}) = \lambda/2 - 1 = 0$ if and only if $\lambda = 2$, so we may have a bifurcation point when $hf'(u^*) = 2$. In order to confirm this we consider the third-order SDIRK method,

$$\begin{array}{c|ccc} 1/3 & 1/3 & & \\ 1/2 & 1/6 & 1/3 & \\ \hline 1 & 2 & -4/3 & 1/3 \\ \hline & 3/4 & 0 & 1/4 \end{array} \quad (3.21)$$

Then

$$u_{n+1} = u_n + \frac{h}{4} (3f(z_1) + f(z_3)), \quad (3.22)$$

where

$$\begin{aligned} z_1 &= u_n + \frac{h}{3} f(z_1), \\ z_2 &= u_n + h \left(\frac{1}{6} f(z_1) + \frac{1}{3} f(z_3) \right), \\ z_3 &= u_n + h \left(2f(z_1) - \frac{4}{3} f(z_2) + \frac{1}{3} f(z_3) \right), \end{aligned} \quad (3.23)$$

with $\xi_i = f(z_i)$, $i = 1, 2, 3$.

We have studied the fixed points of (3.22) with z_1, z_2, z_3 satisfying (3.23) using again the continuation package AUTO in the case $f(u) = u(u - 1)$. Now $u^* = 1$ is unstable because $f'(1) = 1$, and the bifurcation must be at $h = 2$. In Fig. 7 we have plotted the variables u, z_1, z_2 , and z_3 against the parameter h ; the bifurcation point for $h = 2$ is clearly seen.

For $\gamma = \frac{1}{2}$, $p_B(\lambda, \frac{1}{2}) = -\lambda^2/2 + \lambda - 1 = 0 \Leftrightarrow \lambda = 3 \pm \sqrt{3}$ and for the third-order SDIRK method,

$$\begin{array}{c|ccc} 1/2 & 1/2 & & \\ 2/3 & 1/6 & 1/2 & \\ \hline 1 & 3/2 & -1 & 1/2 \\ \hline & 2 & -3/2 & 1/2 \end{array} \quad (3.24)$$

we have found Fig. 8 with bifurcations at $h = 1.267949$ and $h = 4.732051$.

DEFINITION 3.4. A Runge–Kutta method (3.1), (3.2) is *B-regular* if $\det(B(\lambda)) \neq 0$ for each $\lambda \neq 0$.

Assume now that a given method is B-irregular, so that there exists $\lambda^* \neq 0$ such that $\det(B(\lambda^*)) = 0$, and assume that

$$\lambda^* \neq \frac{1}{\lambda_j}, \quad j = 1, \dots, s \quad (3.25)$$

where $\lambda_1, \dots, \lambda_s$ are the eigenvalues of the matrix A . Then from (3.11a) $\eta = (I - \lambda^*A)^{-1}\mathbf{1}$ and (3.11b) is

$$\mathbf{b}^T(I - \lambda^*A)^{-1}\mathbf{1} = \frac{1}{\lambda^*} (R(\lambda^*) - 1) = 0, \quad (3.26)$$

where $R(\lambda)$ is the stability function of the method (Hairer and Wanner [18]). Then if exist $\lambda^* \neq 0$ (for $\lambda^* = 0$ (3.11) has no solution by consistency) satisfying (3.25) such that $R(\lambda^*) = 1$, $\det(B(\lambda^*)) = 0$ and the method is B-irregular. Also, since $\text{rank } B(\lambda^*) = s$ is a simple root and there exists bifurcation point, spurious equilibria and the method is irregular.

THEOREM 3.5. *The condition $R(\lambda) \neq 1$ for $\lambda \neq 0$ satisfies (3.25) is necessary to the B-regularity and regularity of the Runge–Kutta methods.*

When $R(\lambda)$ is irreducible, so that the poles of $R(\lambda)$ are exactly the zeros of $\det(I - \lambda A)$, $R(\lambda) = 1$ implies (3.25), then $\det(B(\lambda^*)) = 0$, and there exists a bifurcation point.

We next study the case when $\det(B(\lambda^*)) = 0$ with $\lambda^* = 1/\lambda_j$ for some eigenvalue of the matrix A .

LEMMA 3.6. *Set*

$$Q = \begin{pmatrix} P & \mathbf{1} \\ \mathbf{b}^T & 0 \end{pmatrix}, \quad (3.27)$$

where P is a $s \times s$ singular matrix, $\mathbf{b} = (b_1, \dots, b_s)^T$, and $\mathbf{1} = (1, \dots, 1)^T$:

- (i) If $\text{rank } P = s - 1$, then $\det Q = 0$ if and only if $\mathbf{b}^T \xi = 0$ or $\eta^T \mathbf{1} = 0$ with $P\xi = 0$ and $\eta^T P = 0$.
- (ii) If $\text{rank } P \leq s - 2$ then $\det Q = 0$.

Proof. (i) If $\text{rank } P = s - 1 \exists M, N$ not singular $s \times s$ matrix such that

$$MPN = \begin{pmatrix} 1 & & & \\ & \ddots & & \\ & & 1 & \\ & & & 0 \end{pmatrix} = \begin{pmatrix} I_{s-1} & \\ & 0 \end{pmatrix}$$

(Gantmakher [11]). Then the matrix

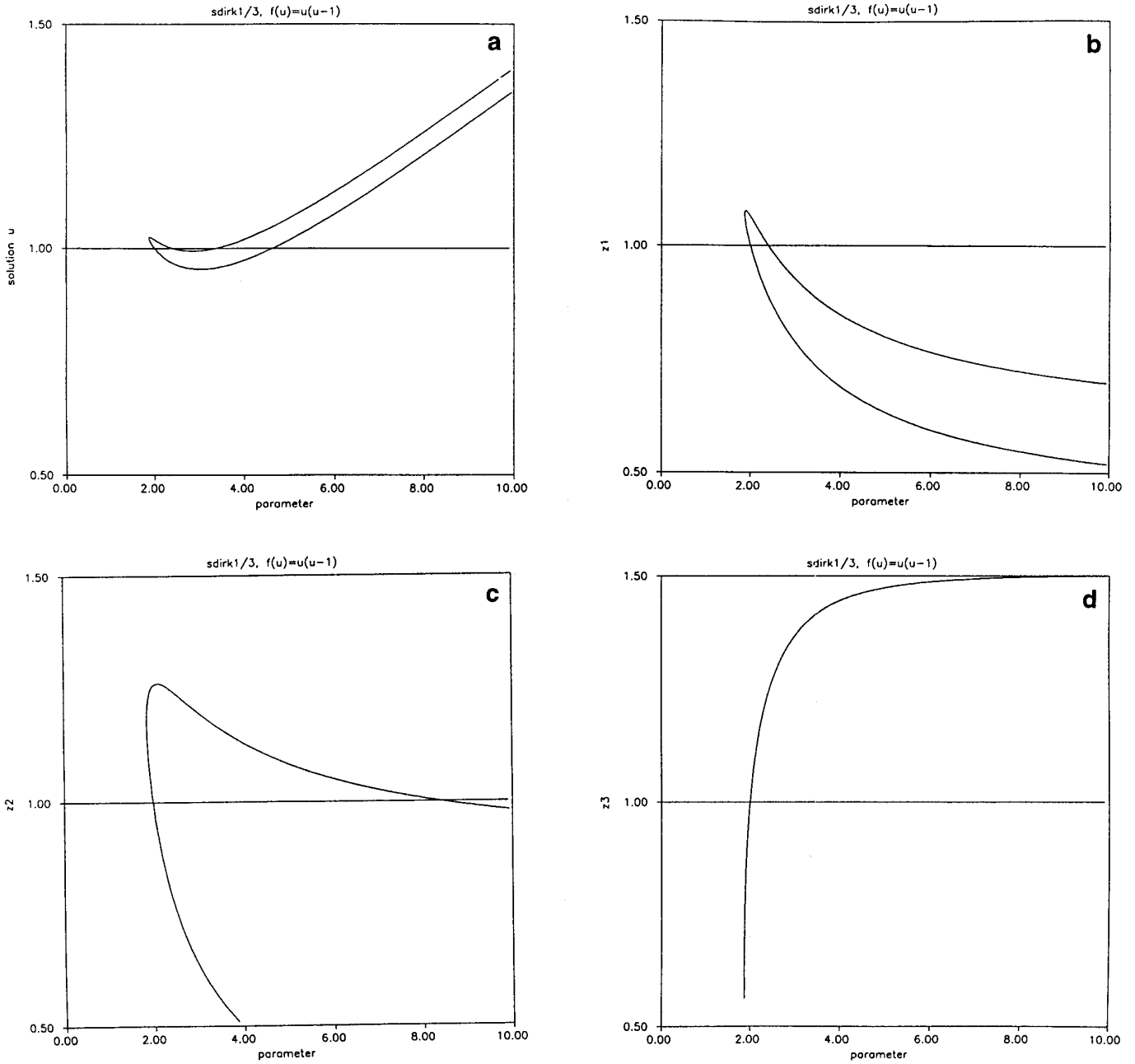


FIGURE 7

$$\begin{pmatrix} M & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix}, \begin{pmatrix} N & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix}$$

$$= \begin{pmatrix} I_{s-1} & \mathbf{0} & \vdots \\ \mathbf{0}^T & 0 & \eta^T \mathbf{1} \\ \dots & B^T \xi & 0 \end{pmatrix},$$

is two regular $(s + 1) \times (s + 1)$ matrices and

$$\begin{pmatrix} M & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \begin{pmatrix} P & \mathbf{1} \\ \mathbf{b}^T & 0 \end{pmatrix} \begin{pmatrix} N & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} = \begin{pmatrix} MPN & M\mathbf{1} \\ \mathbf{b}^T N & 0 \end{pmatrix}$$

where $P\xi = 0$ and $\eta^T P = 0$ and the proof is straightforward.

(ii) If $\text{rank } P \leq s - 3 \Rightarrow \text{rank } Q \leq s - 1 \Rightarrow \det Q = 0$.

If $\text{rank } P = s - 2$ the proof is by absurdum reduction. Let us suppose that $\det Q \neq 0$:

$$\det Q = \begin{vmatrix} p_{1,1} & \cdots & p_{1,s} & 1 \\ \vdots & \ddots & \vdots & \vdots \\ p_{s,1} & \cdots & p_{s,s} & 1 \\ b_1 & \cdots & b_s & 0 \end{vmatrix}$$

$$= \begin{vmatrix} p_{1,1} & \cdots & p_{1,s} & 1 \\ p_{2,1} - p_{1,1} & \cdots & p_{2,s} - p_{1,s} & 0 \\ \vdots & \ddots & \vdots & \vdots \\ p_{s,1} - p_{1,1} & \cdots & p_{s,s} - p_{1,s} & 0 \\ b_1 & \cdots & b_s & 0 \end{vmatrix}$$

$$= \pm \begin{vmatrix} p_{2,1} - p_{1,1} & \cdots & p_{2,s} - p_{1,s} \\ \vdots & \ddots & \vdots \\ p_{s,1} - p_{1,1} & \cdots & p_{s,s} - p_{1,s} \\ b_1 & \vdots & b_s \end{vmatrix}$$

$$\neq 0 \Rightarrow \text{rank } P \geq s - 1,$$

in contradiction to the hypothesis and then $\det Q = 0$. ■

We now conclude the following theorem which characterizes all B-regular Runge–Kutta methods.

THEOREM 3.7. *A Runge–Kutta method is B-regular if and only if*

(c₁) $R(\lambda) \neq 1$ for $\lambda \neq 0$.

(c₂) *Every eigenvalue of A has a one-dimensional null-space and its right and left eigenvectors satisfy $\mathbf{b}^T \xi \neq 0$ and $\eta^T \mathbf{1} \neq 0$.*

EXAMPLE 3.8. The third-order SDIRK method (3.21) of Fig. 7 has no bifurcation at $\lambda = 3$ because $\text{rank}(I - 3A) = 3 - 1 = 2$ and the left and right eigenvectors are $\eta = (\eta_1, 0, 0)^T$ and $\xi = (0, 0, \xi_s)^T$, and $\mathbf{b}^T \xi = \frac{1}{4} \xi_s \neq 0$, $\eta^T \mathbf{1} = \eta_1 \neq 0$.

EXAMPLE 3.9. Consider the third-order SDIRK method

$$\begin{array}{c|ccc} \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{2} + \frac{\sqrt{3}}{6} & & \\ \frac{1}{2} & -\frac{\sqrt{3}}{6} & \frac{1}{2} + \frac{\sqrt{3}}{6} & \\ 1 & \frac{1}{2} - \frac{\sqrt{3}}{6} & 0 & \frac{1}{2} + \frac{\sqrt{3}}{6} \\ \hline & -\frac{\sqrt{3}}{2} - \frac{1}{2} & \frac{\sqrt{3}}{3} + 1 & \frac{\sqrt{3}}{6} + \frac{1}{2} \end{array}, \quad (3.28)$$

with $\gamma = 1/2 + \sqrt{3}/6 \doteq 0.788675$ and

$$\det(B(\lambda)) = -\lambda^2 \left(\frac{\sqrt{3}}{4} + \frac{5}{12} \right) + \lambda \left(\frac{\sqrt{3}}{2} + 1 \right) - 1. \quad (3.29)$$

Now for $\lambda^* = 1/\gamma = 6/(3 + \sqrt{3})$ $\text{rank}(I - \lambda^*A) = s - 2 = 1$, and there is bifurcation because $\text{rank } B(\lambda^*) = 3$. Figure 9 agrees with this prediction, we obtain exactly two bifurcation points at $h = 0.9282108$ and $h = 1.267876 \doteq 1/0.788675$, where $\det(B(\lambda)) = 0$.

To sum up, in this section we have computed branches of spurious fixed points in Runge–Kutta methods connected with bifurcation points of essential fixed points u^* at $h^* = \lambda^*/f'(u^*)$, where λ^* is in one of the three following cases:

(i) $R(\lambda^*) = 1$ with $\lambda^* \neq 1/\lambda_j$, $j = 1, \dots, s$, eigenvalues of A.

(ii) $\lambda^* = 1/\lambda_j$ with λ_j eigenvalue of A and $\text{rank}(I - \lambda^*A) = s - 1$ and $\mathbf{b}^T \xi = 0$ or $\eta^T \mathbf{1} = 0$, where $(I - \lambda^*A)\xi = 0$ and $\eta^T(I - \lambda^*A) = 0$.

(iii) $\lambda^* = 1/\lambda_j$ with λ_j eigenvalue of A and $\text{rank}(I - \lambda^*A) \leq s - 2$, and $\text{rank } B(\lambda^*) = s - p$ with p an even number, which means λ^* is odd multiplicity.

In fact, the situation now is the following: the R-regularity implies that the bifurcation points of the essential fixed points do not exist and in the opinion of the author the method is regular. “I admit that each and every thing remains in its state until there is reason for change” (Leibnitz). The difference between B-regularity and regularity is when $\text{rank}(I - \lambda^*A) \leq s - 2$ and $\text{rank } B(\lambda^*) = s - p$ with p an odd number, then λ^* has even multiplicity and may exist or not bifurcation point.

Hairer, Iserles, and Sanz-Serna [17] have proved that the maximal order of Runge–Kutta methods such that $R(\lambda) \neq 1$ whenever $\lambda \neq 0$ is $p \leq s + 2$ if s , the number of stages, is even and $p \leq s + 1$ if s is odd. However, they did not know regular Runge–Kutta methods of order $p > 4$. Iserles [20] found regular methods of order 4, including the method of Hammer and Hollingsworth (Lambert [23]), and these methods are B-regular too (Example 3.2).

If we look for B-regular Runge–Kutta methods of order 5, we have to consider $s = 4$ and methods with stability function $R(\lambda)$ a rational approximation to e^λ of order ≥ 5 . This approximation cannot be a Padé approximation (Hairer, Iserles, and Sanz-Serna [17]).

Nevertheless, the situation is not quite so pessimistic because if there exists λ^* such that $R(\lambda^*) = 1$ or an eigenvalue of A does not satisfy condition (c₂), in order that a bifurcation point exist, step h must satisfy

$$h \cdot \mathfrak{S}f'(u^*) = \mathfrak{S}\lambda^*, \quad (3.30)$$

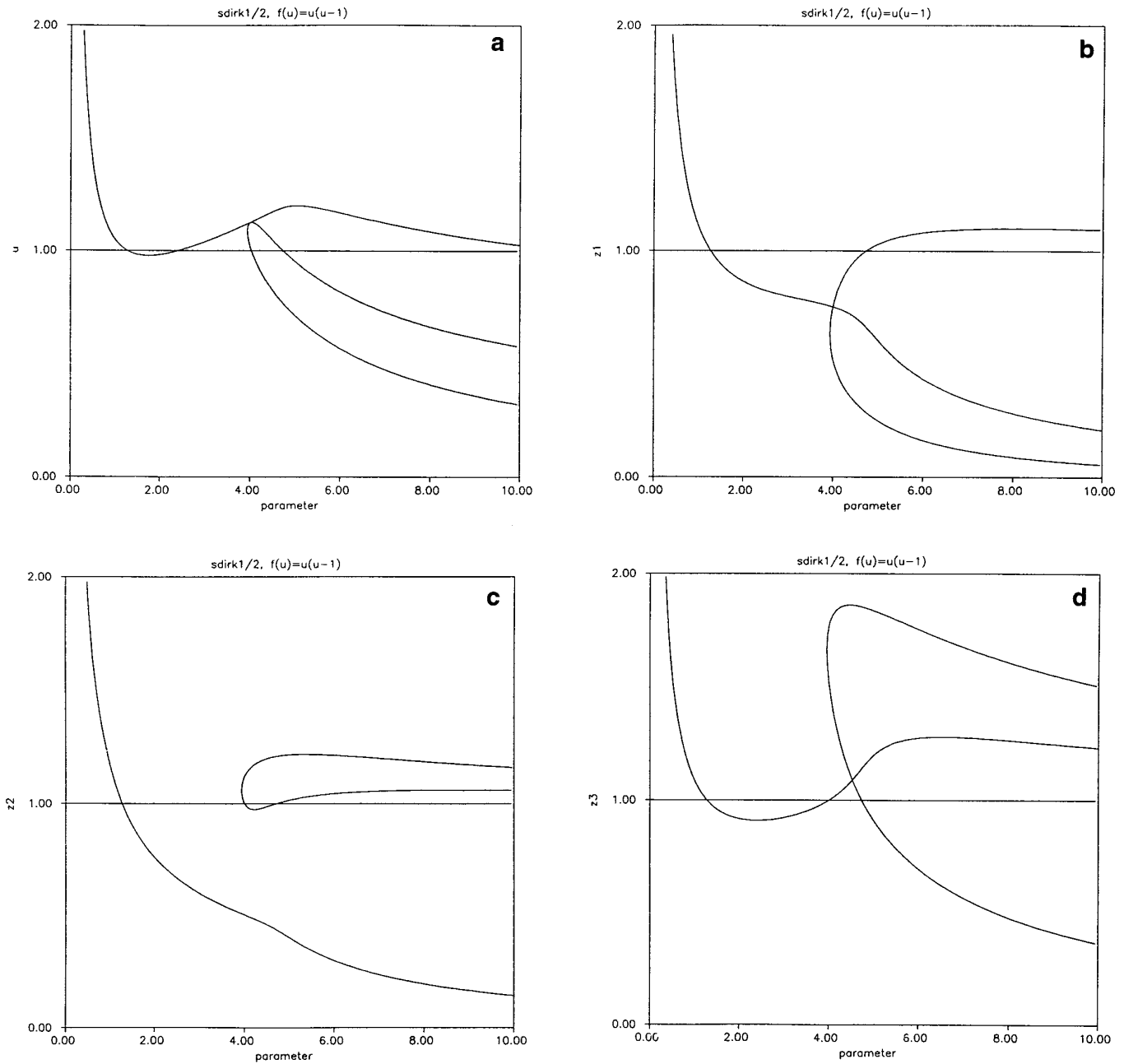


FIGURE 8

$$h \cdot \Re f'(u^*) = \Re \lambda^*,$$

where $\Re \lambda^*$ and $\Im \lambda^*$ mean the real and imaginary part of the complex number λ^* . Therefore, each B-irregular Runge–Kutta method has bifurcation from u^* and branches of spurious fixed points exist *only* for those initial value problems such that $f'(u^*)$ solve (3.30) for some fixed point u^* .

4. R-REGULARITY AND BR-REGULARITY OF RUNGE–KUTTA METHODS

We are now going to consider the onset of real spurious fixed points for Runge–Kutta methods. When studying some real dynamical system using a numerical method with real floating-point arithmetic, we only detect real essential fixed points and spurious real fixed points. Our aim is to prevent the spurious behaviour.

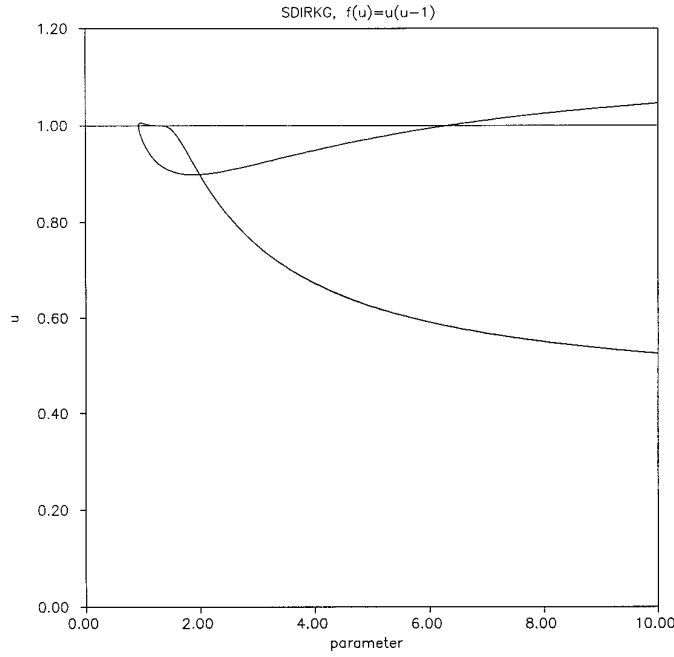


FIGURE 9

We say that a Runge–Kutta method (3.3) is *R-regular* (R real), if for all $h > 0$ and all initial value problem (1.1), every real zero of ϕ is a zero of f . We say that (3.3) is *BR-regular* if $\det(B(\lambda)) \neq 0$, $\lambda \neq 0$, $\lambda \in \Re$. It is then clear that

$$R\text{-regularity} \Rightarrow BR\text{-regularity} \Rightarrow R(\lambda) \neq 1, \quad \forall \lambda \neq 0, \lambda \in \Re. \quad (4.1)$$

While *R-regular* methods do not have real spurious fixed points, *BR-regular* methods do not have real bifurcation points, whenever $f'(u^*)$ is real $\det(B(hf'(u^*))) \neq 0$.

The following theorem shows that there is no nonconfluent Runge–Kutta method of two stages and order 2 (3.14) that is *R-regular* but which is not regular.

THEOREM 4.1. *A 2 stages non-confluent Runge–Kutta method of order $p \geq 2$ is R-regular if and only if it is regular.*

Proof. Obviously regularity implies *R-regularity*.

Assume that the method is *R-regular*. Because the method is at least of second order, $R(\lambda)$ is of the form

$$R(\lambda) = \frac{1 + (1 + \alpha_1)\lambda + (\frac{1}{2} + \alpha_1 + \alpha_2)\lambda^2}{1 + \alpha_1\lambda + \alpha_2\lambda^2}$$

and $R(\lambda) \neq 1$ for real $\lambda \neq 0$. Then,

$$\lambda + (\frac{1}{2} + \alpha_1)\lambda^2 \neq 0, \quad \lambda \neq 0, \lambda \in \Re,$$

and this is possible if and only if $\alpha_1 = -\frac{1}{2}$. Since $\alpha_1 = -\text{trace } A$ (Hairer and Wanner [18]), $\text{trace } A = \frac{1}{2}$, which is the characterization of regularity of Iserles [20].

Let us now consider the *BR-regularity* of Runge–Kutta methods, according to Section 3.

THEOREM 4.2. *A Runge–Kutta method is BR-regular if and only if*

$$(cr_1) \quad R(\lambda) \neq 1, \lambda \neq 0, \lambda \in \Re.$$

(*cr*₂) *Every real eigenvalue of A has a one-dimensional null-space and its right and left eigenvectors satisfy $\mathbf{b}^T \boldsymbol{\xi} \neq 0$ and $\boldsymbol{\eta}^T \mathbf{1} \neq 0$, respectively.*

The question we now address is the construction of a *BR-regular* Runge–Kutta method of order five.

A useful formula for the stability function of a Runge–Kutta method is

$$R(\lambda) = \frac{P(\lambda)}{Q(\lambda)} = \frac{\det(I - \lambda A + \lambda \mathbf{1} \cdot \mathbf{b}^T)}{\det(I - \lambda A)} \quad (4.2)$$

(Hairer and Wanner [18]). If we want a *BR-regular* method of order 5 and three stages, we must look for a Padé approximations such that $R(\lambda) \neq 1$, $\lambda \neq 0$, $\lambda \in \Re$, and $Q(\lambda) \neq 0$, $\lambda \in \Re$. The (3,2)-Padé approximation

$$R_{3,2}(\lambda) = \frac{P_3(\lambda)}{Q_2(\lambda)} = \frac{1 + \frac{3}{5}\lambda + \frac{3}{20}\lambda^2 + \frac{1}{60}\lambda^3}{1 - \frac{2}{5}\lambda + \frac{1}{20}\lambda^2} \quad (4.3)$$

satisfies these requirements, and the problem is reduced to finding a 3-stage Runge–Kutta method with stability function (4.3) and order 5.

We consider the method

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ c_2 & c_2 - a_{2,2} - a_{2,3} & a_{2,2} & a_{2,3} \\ c_3 & c_3 - a_{3,2} - a_{3,3} & a_{3,2} & a_{3,3} \\ \hline & 1 - b_2 - b_3 & b_2 & b_3 \end{array} \quad (4.4)$$

with

$$a_{2,3} = \left(\frac{2}{5} - a_{2,2}\right) \frac{a_{2,2}}{a_{3,2}} - \frac{1}{20a_{3,2}}, \quad (4.5)$$

$$a_{3,3} = \frac{2}{5} - a_{2,2}. \quad (4.6)$$

The construction relies on the simplifying assumptions

$$B(p): \sum_{i=1}^s b_i c_i^{q-1} = \frac{1}{q},$$

$$q = 1, \dots, p, \tag{4.7}$$

$$C(\eta): \sum_{j=1}^s a_{i,j} c_j^{q-1} = \frac{c_i^q}{q},$$

$$i = 1, \dots, s, q = 1, \dots, \eta, \tag{4.8}$$

$$D(\zeta): \sum_{i=1}^s b_i c_i^{q-1} a_{i,j} = \frac{b_j}{q} (1 - c_j)^q,$$

$$j = 1, \dots, s, q = 1, \dots, \zeta. \tag{4.9}$$

The importance of these conditions is seen from the following well-known theorem.

THEOREM 4.3. (Butcher, 1964). *If the coefficient b_i , c_i , $a_{i,j}$ satisfy $B(p)$, $C(\eta)$, $D(\zeta)$ with $p \leq \eta + \zeta + 1$, $p \leq 2\eta + 2$, then the method is of order p .*

In our situation, $s = 3$ and $p = 5$, and we consider $\eta = \zeta = 2$ so that we have to impose $B(5)$, $C(2)$, $D(2)$.

The conditions $B(5)$ mean that the quadrature formula is of order 5, and since $c_1 = 0$,

$$\begin{aligned} b_1 + b_2 + b_3 &= 1, \\ b_2 c_2 + b_3 c_3 &= \frac{1}{2}, \\ b_2 c_2^2 + b_3 c_3^2 &= \frac{1}{3}, \\ b_2 c_2^3 + b_3 c_3^3 &= \frac{1}{4}, \\ b_2 c_2^4 + b_3 c_3^4 &= \frac{1}{5}. \end{aligned} \tag{4.10}$$

Then, b_1, b_2, b_3 are the weights and c_2, c_3 the nodes of the Radau quadrature formula of order 5

$$\begin{aligned} c_2 &= \frac{6 - \sqrt{6}}{10}, \\ c_3 &= \frac{6 + \sqrt{6}}{10}, \\ b_1 &= \frac{1}{9}, \\ b_2 &= \frac{16 + \sqrt{6}}{36}, \\ b_3 &= \frac{16 - \sqrt{6}}{36}. \end{aligned} \tag{4.11}$$

Now, from $C(2)$, (4.5), and (4.6) we get the solution

$$a_{2,2} = \frac{8647}{39231}, \quad a_{3,2} = \frac{4960}{8581}. \tag{4.12}$$

We are thus led to the following method

0	0	0	0	
$\frac{6 - \sqrt{6}}{10}$	$\frac{1960}{12839}$	$\frac{8647}{39231}$	$-\frac{1104}{61261}$	
$\frac{6 + \sqrt{6}}{10}$	$\frac{3197}{36604}$	$\frac{4960}{8581}$	$\frac{11513}{64108}$	(4.13)
.	.	.	.	
.	$\frac{1}{9}$	$\frac{16 + \sqrt{6}}{36}$	$\frac{16 - \sqrt{6}}{36}$	

In order to prove (4.13) has order 5, we must show that the coefficients satisfy $D(2)$. We use the W-transformation (Hairer and Wanner [18]).

Let $P_i(x)$ be the shifted Legendre polynomials normalized and let $W = (w_{i,j})$ be defined by $w_{i,j} = P_{j-1}(c_i)$, $i, j = 1, 2, 3$, and the matrix

$$X_G = \begin{pmatrix} -\frac{1}{2} & -\xi_1 & 0 \\ \xi_1 & 0 & -\xi_2 \\ 0 & \xi_2 & -\frac{1}{10} \end{pmatrix}, \tag{4.14}$$

where $\xi_k = 1/2\sqrt{4k^2 - 1}$ for $k = 1, 2$.

The main theorem (Hairer and Wanner [18, Theorem 5.11]) says that the conditions $D(2)$ are satisfied if and only if the first two rows for the matrix $X = W^{-1}AW$ are those of X_G , where A is the coefficient matrix for the method. With the help again of algebraic manipulation package we confirm that (4.13) is of order five and the method we are searching. In fact, we have applied (4.13) to a set of examples with real steady states, and we have never found spurious fixed points.

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