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Spurious solutions of numerical methods for initial value problems

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It is well known that some numerical methods for initial value problems admit spurious limit sets. Here the existence and behaviour of spurious solutions of Runge–Kutta, linear multistep and predictor-corrector methods are studied in the limit as the step-size $h \to 0$. In particular, it is shown that for ordinary differential equations defined by globally Lipschitz vector fields, spurious fixed points and period 2 solutions cannot exist for h arbitrarily small, whilst for locally Lipschitz vector fields, spurious solutions may exist for h arbitrarily small, but must become unbounded as $h \to 0$. The existence of spurious solutions is also studied for vector fields merely assumed to be continuous, and an example is given, showing that in this case spurious solutions may remain bounded as $h \to 0$. It is shown that if spurious fixed points or period 2 solutions of continuous problems exist for h arbitrarily small, then as $h \to 0$ spurious solutions either converge to steady solutions of the underlying differential equation or diverge to infinity. A necessary condition for the bifurcation spurious solutions from $h = 0$ is derived. To prove the above results for implicit Runge–Kutta methods, an additional assumption on the iteration scheme used to solve the nonlinear equations defining the method is needed; an example of a Runge-Kutta method which generates a bounded spurious solution for a smooth problem with h arbitrarily small is given, showing that such an assumption is necessary. It is also shown that an Adams–Bashforth/Adams–Moulton predictor-corrector method in PC^m implementation can generate spurious fixed point solutions for any m.

1. Introduction

In this paper we are concerned with the solution of the autonomous initial value problem: find $\mathbf{y} \in \mathscr{R}^m$ satisfying

$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} = \mathbf{f}(\mathbf{y}) \quad \text{for} \quad t \geqslant 0 \quad \text{and} \quad \mathbf{y}(0) = \mathbf{y}_0 \tag{1.1}$$

where $\mathbf{f}: \mathscr{R}^m \to \mathscr{R}^m$. Continuity conditions on $\mathbf{f}$ will be stated where required.

Often (1.1) cannot be solved in closed form and a numerical method is used to replace the continuous system by a finite dimensional map. It is then essential to consider: *What is the relationship between the flow associated with the differential equation* (1.1) *and the flow associated with the map used to model the system numerically*? Often it is the asymptotic behaviour of (1.1) which is of interest, and so in this paper we will compare the asymptotic behaviour of (1.1) and its numerical counterpart.

Standard convergence results for numerical methods give error bounds of the form $e^{cT}h^p$ for individual trajectories, where h is the step-size, p is the order of the method, c is a constant (typically positive) and T is the length of the time interval over which the integration occurs. Such estimates can be used to show that, on a compact time interval, the trajectory associated with the map converges to the corresponding trajectory of the continuous system as $h \to 0$. However if we wish to compare the asymptotic features of the dynamical system and the associated map such estimates become useless as $T \to \infty$ (except in rare cases where $c < 0$), and methods for initial value problems which are convergent in finite time do not necessarily yield the same asymptotic behaviour as the underlying differential equation for small fixed step-size.

The possible asymptotic states are given by the α and ω limit sets. Typically these contain fixed points, periodic orbits, quasi-periodic orbits and strange-attractors. See [4] for a complete description of these objects. The simplest limit sets are fixed points (also called steady solutions). If the fixed points of the continuous and numerical systems are different, then clearly so will be the dynamics of the two systems, thus for a numerical method to reproduce the correct asymptotic behaviour it is essential that it has the same set of fixed points as the underlying continuous problem (1.1) which it is approximating.

Runge–Kutta or linear multistep methods are often used to obtain a numerical solution of (1.1). Iserles [7] showed that these methods retain all the fixed points of (1.1), however Runge–Kutta methods (but not linear multistep methods) may have additional spurious fixed points, not corresponding to fixed points of the continuous system, and thus may display incorrect dynamics.

It is also possible for some numerical methods to converge to solutions of the form $\mathbf{y}_{2n} = \mathbf{u}$, $\mathbf{y}_{2n+1} = \mathbf{v}$, where $\mathbf{u} \neq \mathbf{v}$. This is known as a *period* 2 *solution* (or 2-*cycle* or *sawtooth solution*). Such periodic motion on the grid scale must be spurious. If the 2-cycle is stable then it will attract a certain subset of initial conditions, whilst if it is unstable it has been observed [11] that the unstable manifold of the spurious solution is often connected to infinity, thus destroying any global attractor which may exist for (1.1). Thus although period 2 solutions are easy to recognise as spurious, it is preferable to use methods which do not produce this behaviour.

The observations above led to the following definitions, which are reproduced from [8].

DEFINITION 1.1 A numerical method for (1.1) which does not admit spurious fixed points is said to be *regular of degree* 1, denoted $R^{[1]}$. A method which is not $R^{[1]}$ is said to be *irregular of degree* 1, denoted $IR^{[1]}$.

DEFINITION 1.2 A numerical method for (1.1) which does not admit period two solutions is said to be *regular of degree* 2, denoted $R^{[2]}$. A method which is not $R^{[2]}$ is said to be *irregular of degree* 2, denoted $IR^{[2]}$.

We will also use the notation $R^{[1,2]}$ to denote a method which is $R^{[1]}$ and $R^{[2]}$, etc. Examples of spurious fixed point and period 2 solutions, and their effect on the dynamics of the numerical map can be found in [3, 7, 8, 10, 11, 12]. These spurious solutions often bifurcate from the linear stability limit, but it should be noted that they can persist for arbitrarily small values of the step-size h, and thus incorrect asymptotic behaviour can be observed at step-sizes used in practical implementations.

A thorough study of regular Runge–Kutta and linear multistep methods has been conducted in [5, 7, 8, 9, 12]. Iserles [7] presents examples of spurious steady solutions of Runge–Kutta, linear multistep and predictor-corrector methods arising from Riccati equations, and also shows that all linear multistep methods are $R^{[1]}$. Stuart and Peplow [12] classify the $R^{[1,2]}$ one step linear multistep methods, and study the period 2 solutions of $IR^{[2]}$ methods. That paper was also the first to consider the existence of spurious solutions of irregular methods in the limit as $h \to 0$. It was shown that if $\mathbf{f} \in C^1(\mathcal{R}^m, \mathcal{R}^m)$, period 2 solutions of $IR^{[2]}$ one step linear multistep methods become unbounded as $h \to 0$, if they exist for h arbitrarily small. This result, which is a special case of Theorem B(c)(ii) below, inspires the approach of the current work. Hairer, Iserles and Sanz-Serna [5] conduct a systematic study of the spurious equilibria of Runge–Kutta methods, and in particular classify all the $R^{[1]}$ Runge–Kutta methods by means of a recursive test. Iserles, Peplow and Stuart [8] present a unified theory of spurious solutions based on local bifurcation theory, using the step-size h as the bifurcation parameter. Amongst many other results they show that the maximum order of a $R^{[1,2]}$ Runge–Kutta method is 2, and that the recursive test of [5] can be used to classify these methods. Also in that paper all the $R^{[2]}$ linear multistep methods are identified and the regularity properties of a class of predictor-corrector methods are studied. In [9] Iserles and Stuart consider $R^{[1,2]}$ linear multistep methods further, and a modification of the backward differentiation formulae which generates such methods is proposed.

Other considerations mean that (1.1) is often numerically integrated using a method which is not $R^{[1,2]}$. For example the highest possible order of a $R^{[1,2]}$ Runge–Kutta method is 2, and Hairer *et al.* [5] proved that the Forward Euler method is the only $R^{[1]}$ explicit Runge–Kutta method. If a method which is not $R^{[1,2]}$ is used, then spurious solutions may exist, and to ensure good numerical reproduction of the dynamics of (1.1) it is necessary to study the existence of spurious solutions in irregular methods. This approach, complimentary to the study of regular methods *per se*, will be followed in this paper.

Throughout we will be concerned with fixed time stepping methods, but will treat the step-size h as a parameter and consider the existence of spurious fixed point and period 2 solutions in the limit as $h \to 0$. Simple continuity conditions will be applied to $\mathbf{f}$ in (1.1), which will allow us to derive results on the possible existence and boundedness of spurious solutions in the limit as $h \to 0$. The main results are stated below.

THEOREM A If a numerical approximation to (1.1) is obtained using either;

(a) an explicit Runge–Kutta method,

(b) an implicit Runge–Kutta method, where (2.1) is solved using the iteration (2.11),

(c) an Adams–Bashforth/Adams–Moulton predictor-corrector method in PC^m implementation (see Section 5),

then

(i) if $\mathbf{f}$ is globally Lipschitz spurious fixed points cannot exist for h arbitrarily small,

(ii) if $\mathbf{f}$ is locally Lipschitz, and in particular if $\mathbf{f} \in C^1(\mathcal{R}^m, \mathcal{R}^m)$, and spurious fixed points exist for h arbitrarily small, then these spurious fixed points tend to infinity, in norm, as $h \to 0$,

(iii) if $\mathbf{f} \in C(\mathcal{R}^m, \mathcal{R}^m)$ and a continuous branch $\tilde{\mathbf{y}}(h)$ of fixed solutions of the numerical method exists for h sufficiently small, then as $h \to 0$, $\|\tilde{\mathbf{y}}(h)\| \to \infty$ or $\|\mathbf{f}(\tilde{\mathbf{y}}(h))\| \to 0$. If furthermore the zeros of $\mathbf{f}$ are isolated then $\|\mathbf{f}(\tilde{\mathbf{y}}(h))\| \to 0$ implies $\tilde{\mathbf{y}}(h) \to \bar{\mathbf{y}}$, a fixed point of (1.1),

(iv) if a spurious fixed point solution bifurcates from $\tilde{\mathbf{y}}$ at $h = 0$ then either $\mathbf{f}$ is not continuous at $\tilde{\mathbf{y}}$, or, $\mathbf{f}(\tilde{\mathbf{y}}) = 0$ and $\mathbf{f}$ is not Lipschitz at $\tilde{\mathbf{y}}$.

THEOREM B If a numerical approximation to (1.1) is obtained using either;

(a) an explicit Runge–Kutta method,

(b) an implicit Runge–Kutta method, where (2.1) is solved using the iteration (2.11),

(c) a zero-stable linear multistep method of the form (4.1), with $\rho(-1) \neq 0$,

then

(i) if $\mathbf{f}$ is globally Lipschitz period 2 solutions cannot exist for h arbitrarily small,

(ii) if $\mathbf{f}$ is locally Lipschitz, and in particular if $\mathbf{f} \in C^1(\mathcal{R}^m, \mathcal{R}^m)$, and a period 2 solution $(\mathbf{u}(h), \mathbf{v}(h))$ exists for h arbitrarily small, then $\mathbf{u}(h)$, $\mathbf{v}(h)$ both tend to infinity, in norm, as $h \to 0$,

(iii) if $\mathbf{f} \in C(\mathcal{R}^m, \mathcal{R}^m)$ and a continuous branch $(\mathbf{u}(h), \mathbf{v}(h))$ of period 2 solutions of the numerical method exists for h arbitrarily small, then as $h \to 0$, $\|\mathbf{u}(h)\|$, $\|\mathbf{v}(h)\|$ both tend to infinity, or $\|\mathbf{f}(\mathbf{u}(h))\|$, $\|\mathbf{f}(\mathbf{v}(h))\|$ and $\|\mathbf{u}(h) - \mathbf{v}(h)\| \to 0$. If furthermore the zeros of $\mathbf{f}$ are isolated then $\|\mathbf{f}(\mathbf{u}(h))\| \to 0$ implies $\mathbf{u}(h)$, $\mathbf{v}(h)$ tend to $\bar{\mathbf{y}}$, a fixed point of (1.1),

(iv) if a period 2 solution bifurcates from $\tilde{\mathbf{y}}$ at $h = 0$ then either $\mathbf{f}$ is not continuous at $\tilde{\mathbf{y}}$, or, $\mathbf{f}(\tilde{\mathbf{y}}) = 0$ and $\mathbf{f}$ is not Lipschitz at $\tilde{\mathbf{y}}$.

THEOREM C Every Adams–Bashforth/Adams–Moulton predictor-corrector method in PC^m mode is $IR^{[1]}$.

The proofs of the above results can be found in the following sections, where sufficient bounds on the step-size h to prevent spurious solutions in the case where $\mathbf{f}$ is globally Lipschitz are also given, and many other results can also be found.

In Section 2 we develop the theory for spurious fixed point solutions of Runge–Kutta methods. In addition to the results above, several corollaries are given, and we also prove that for an implicit method the Runge–Kutta equations (2.1–2) are always soluble for sufficiently small step-size if $\mathbf{f}$ is continuous on some neighbourhood of $\mathbf{y}_n$. Example 2.8 is given which shows that Theorems A and B do not apply to arbitrary solutions of implicit Runge–Kutta methods, and hence that the assumption on the iteration scheme used to solve the implicit equations is necessary.

The theory is extended to cover period 2 solutions of Runge–Kutta and linear multistep methods in Sections 3 and 4. The Runge–Kutta results follow easily from those in Section 2, whilst the linear multistep results follow from Lemma 4.3 which shows that for fixed step-size there is at most one 2-cycle of any linear multistep method passing through any point of $\mathscr{R}^m$. In Example 3.6 a continuous initial value problem that generates bounded spurious solutions for h arbitrarily small is presented, showing that Theorems A(iii) and B(iii) are relevant.

In Section 5 spurious fixed point solutions of predictor-corrector methods are studied. We will show that the fixed point solutions of an Adams–Bashforth/Adams–Moulton predictor-corrector method in PC^m mode correspond to the fixed points of an associated explicit Runge–Kutta method, and hence Theorems A and C apply. We suggest that iterating the corrector to convergence, will give better reproduction of the long term dynamics of (1.1).

We could conclude from Theorems A and B that when $\mathbf{f}$ satisfies a Lipschitz condition, spurious solutions will not degrade the numerical solution if the step-size is sufficiently small. This may not be true because an unstable spurious solution can destroy a global attractor, and even though the spurious solution becomes unbounded as $h \to 0$ the dynamics of the continuous and numerical systems will differ significantly for some initial conditions however small the step-size is. Also initial value problem solvers are often used to draw the phase portraits of a dynamical system, in which case (1.1) must be solved for all possible initial conditions, and the existence of any spurious solution, whether stable or unstable, will degrade the numerical results.

By Theorem A(iv) and B(iv) even for arbitrarily small step-sizes we cannot be sure that a numerical method will produce the correct behaviour in a neighbourhood of a fixed point where $\mathbf{f}$ is not Lipschitz. However it should be noted that the solution of (1.1) itself is not unique in a neighbourhood of such a point.

In seeking to prove general results, no assumption has been made at any stage on the global structure of the nonlinear function $\mathbf{f}$, and hence our results apply to all problems of the form (1.1). It should be noted then, that in some cases and for some methods it can be shown that spurious solutions cannot exist for h arbitrarily small, although $\mathbf{f}$ is not globally Lipschitz, but where some other structure is imposed on the nonlinear term.

Throughout this paper fixed time-stepping methods are studied, and variable time-stepping methods, which are often used in practice, have not been considered. It is hoped that by increasing the understanding of spurious solutions of fixed time-step methods, the analysis of variable time-stepping methods may be facilitated, and the approach of this paper may be directly relevant to such a study.

2. Spurious fixed points of Runge–Kutta methods

In this section the spurious fixed point solutions of explicit and implicit Runge–Kutta methods are considered. Often a Lipschitz continuity condition will be assumed, but a series of ε, δ-arguments will enable us to prove some results when Lipschitz conditions do not apply. A general s-stage Runge–Kutta method may be written as:

$$\mathbf{Y}_i = \mathbf{y}_n + h \sum_{j=1}^{s} a_{i,j}\mathbf{f}(\mathbf{Y}_j), \qquad i = 1, \ldots, s \tag{2.1}$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^{s} b_i\mathbf{f}(\mathbf{Y}_i) \tag{2.2}$$

Here $\mathbf{y}_n$ approximates the exact solution at $t = nh$, $h > 0$. The method is often represented using the Butcher Tableau notation

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b}^T \end{array} \equiv \begin{array}{c|cccc} c_1 & a_{1,1} & a_{1,2} & \cdots & a_{1,s} \\ c_2 & a_{2,1} & a_{2,2} & \cdots & a_{2,s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} \tag{2.3}$$

where $c_j := \sum_{l=1}^{s} a_{j,l}$, $j = 1, \ldots, s$. We will always assume that the method is consistent. This implies that $\sum_{i=1}^{s} b_i = 1$. We will also use the notation

$$l = \max_i \sum_{j=1}^{i-1} |a_{ij}|, \qquad u = \max_i \sum_{j=i}^{s} |a_{ij}|, \tag{2.4}$$

$$a = l + u, \tag{2.5}$$

$$\mathcal{A} = \max_i \sum_{j=1}^{s} |a_{ij}| = \|A\|_\infty, \tag{2.6}$$

and

$$B = \sum_{i=1}^{s} |b_i| \geqslant 1. \tag{2.7}$$

Notice also

$$\mathcal{A} \leqslant a \leqslant 2\mathcal{A}. \tag{2.8}$$

The method (2.1–2) is said to be explicit if

$$a_{i,j} = 0 \qquad \forall 1 \leqslant i \leqslant j \leqslant s$$

and implicit otherwise. The Forward Euler method (2.9) is the simplest and unique one-stage explicit Runge–Kutta method.

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \tag{2.9}$$

The $R^{[1]}$ methods were classified in [5] by a recursive test. A simple classification for explicit methods was found:

THEOREM 2.1 (Hairer, Iserles and Sanz-Serna [5]) A consistent explicit Runge–Kutta method of the form (2.1–2) is $R^{[1]}$ if and only if it produces the same solution sequence as the Forward Euler method (2.9).

The solution to (1.1) is often approximated using a high order explicit Runge–Kutta method. By Theorem 2.1, such a method is necessarily $IR^{[1]}$, and we may expect spurious steady solutions, and hence incorrect dynamics. This motivates our approach of considering the spurious solutions of irregular methods, rather than simply classifying the regular methods.

If the method (2.1–2) is implicit then it will be assumed throughout that the implicit equations (2.1) have been solved exactly. We will prove later that the equations (2.1–2) are always soluble (for sufficiently small step-size) under the continuity conditions that we will impose on $\mathbf{f}$, but that this solution is not necessarily unique. Where the implicit equations are not uniquely soluble, we will need to assume that the equations (2.1) are solved using the iteration (2.11), to enable us to pick a unique solution of these equations. This assumption will be explicitly stated where it is made.

Often $\mathbf{f}$ satisfies a Lipschitz continuity condition. We begin by defining Lipschitz continuity.

DEFINITION 2.2 $\mathbf{f}: \mathcal{R}^m \to \mathcal{R}^m$ is said to be Lipschitz on $X \subset \mathcal{R}^m$ if $\exists L > 0$ such that

$$\|\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{y})\| \leq L\,\|\mathbf{x} - \mathbf{y}\| \qquad \forall \mathbf{x}, \mathbf{y} \in X.$$

Here $\|\cdot\|$ is any norm on $\mathcal{R}^m$. L is said to be the *Lipschitz* constant. $\mathbf{f}$ is said to be *globally Lipschitz* if $\mathbf{f}$ is Lipschitz on $\mathcal{R}^m$. $\mathbf{f}$ is said to be *locally Lipschitz* if $\mathbf{f}$ is Lipschitz on all bounded subsets of $\mathcal{R}^m$. $\mathbf{f}$ is *Lipschitz* at $\mathbf{x} \in \mathcal{R}^m$ if $\mathbf{f}$ is Lipschitz on some neighbourhood of $\mathbf{x}$.

For an implicit method, it is not immediately apparent whether the equations (2.1–2) are soluble. Butcher proved that they are uniquely soluble for sufficiently small step-size if $\mathbf{f}$ is globally Lipschitz.

THEOREM 2.3 (Butcher [1]) If $\mathbf{f}$ is globally Lipschitz with Lipschitz constant L and

$$h < \frac{1}{La} \tag{2.10}$$

then the equations (2.1–2) are uniquely soluble. Furthermore this solution can be found by iteration. Set $\mathbf{Y}_i^0 = \mathbf{y}_n\ \forall i = 1, \ldots, s$ then iterate

$$\mathbf{Y}_i^{N+1} = \mathbf{y}_n + h \sum_{j=1}^{i-1} a_{ij}\mathbf{f}(\mathbf{Y}_j^{N+1}) + h \sum_{j=i}^{s} a_{ij}\mathbf{f}(\mathbf{Y}_j^{N}) \tag{2.11}$$

Then let $\mathbf{Y}_i = \lim_{N\to\infty} \mathbf{Y}_i^N$. This limit exists and defines the solution of (2.1). □

The following Lemma provides a bound on the solution, when a Lipschitz condition is assumed and will enable us to derive directly the nonexistence of spurious solutions in certain regions.

LEMMA 2.4 If $\mathbf{f}$ is Lipschitz on U with Lipschitz constant L, $\mathbf{y}_n \in U$ and $\mathbf{Y}_i \in U\ \forall i$ and

$$h < \frac{1}{L\mathcal{A}} \tag{2.12}$$

then the numerical solution defined by (2.1–2) satisfies

$$\|\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{Y}_i)\| < \frac{L\mathcal{A}h}{1 - L\mathcal{A}h} \|\mathbf{f}(\mathbf{y}_n)\| \qquad \forall i = 1, \ldots, s \tag{2.13}$$

NOTE. The norm in (2.13), and throughout the rest of this paper, can be any norm, but where a particular Lipschitz constant is used, must be consistent with the norm used to define that constant.

Proof. Consider the equations (2.1–2). Let

$$M = \max_j \|\mathbf{f}(\mathbf{Y}_j)\|$$

then

$$\begin{aligned} \|\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{Y}_i)\| &= \left\|\mathbf{f}(\mathbf{y}_n) - \mathbf{f}\left(\mathbf{y}_n + h \sum_{j=1}^{s} a_{i,j}\mathbf{f}(\mathbf{Y}_j)\right)\right\| \\ &\leq Lh \left\|\sum_{j=1}^{s} a_{i,j}\mathbf{f}(\mathbf{Y}_j)\right\| \\ &\leq Lh\mathcal{A}M \end{aligned} \tag{2.14}$$

Hence

$$\|\mathbf{f}(\mathbf{Y}_i)\| \leq Lh\mathcal{A}M + \|\mathbf{f}(\mathbf{y}_n)\|$$

and in particular

$$M \leq Lh\mathcal{A}M + \|\mathbf{f}(\mathbf{y}_n)\|$$

$$(1 - L\mathcal{A}h)M \leq \|\mathbf{f}(\mathbf{y}_n)\|$$

and the result follows from (2.14). □

We now prove the nonexistence of spurious fixed points for h sufficiently small if $\mathbf{f}$ is globally Lipschitz.

THEOREM 2.5 If $\mathbf{f}$ is globally Lipschitz, with Lipschitz constant L, and

$$h < \frac{1}{L\mathcal{A}(1 + B)} \tag{2.15}$$

then the Runge–Kutta method (2.1–2) admits no spurious fixed points when applied to (1.1).

Proof. Suppose there exists a solution of (2.1–2) such that $\mathbf{y}_n = \mathbf{y}_{n+1}$ with $\mathbf{f}(\mathbf{y}_n) \neq 0$. Since $\mathbf{f}$ is globally Lipschitz, Lemma 2.4 applies and (2.13) holds. Now (2.2) implies

$$\sum_{i=1}^{s} b_i\mathbf{f}(\mathbf{Y}_i) = 0 \tag{2.16}$$

and by consistency

$$\begin{aligned}
\|\mathbf{f}(\mathbf{y}_n)\| &= \left\|\sum_{i=1}^{s} b_i \mathbf{f}(\mathbf{y}_n)\right\| \\
&= \left\|\sum_{i=1}^{s} b_i (\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{Y}_i))\right\| \\
&\leqslant B \max_i \|\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{Y}_i)\| \\
&\leqslant \frac{Lh\mathscr{A}B}{1 - hL\mathscr{A}} \|\mathbf{f}(\mathbf{y}_n)\| \quad \text{by (2.13)} \qquad (2.17)
\end{aligned}$$

and since (2.15) holds, (2.17) implies $\|\mathbf{f}(\mathbf{y}_n)\| < \|\mathbf{f}(\mathbf{y}_n)\|$, clearly a contradiction. □

COROLLARY 2.6 If $\mathbf{f} \in C^1(\mathscr{R}^m, \mathscr{R}^m)$ with uniformly bounded Jacobian then there exists $H > 0$ such that if the consistent Runge–Kutta method (2.1–2) is applied to (1.1) with step-size $h < H$, then there are no spurious fixed points. □

There are very few interesting problems of the form (1.1) for which $\mathbf{f}$ is globally Lipschitz, but $\mathbf{f}$ is often locally Lipschitz, and we would like to generalize Theorem 2.5 to this case. The following example modified from an example in [11] shows that this cannot be done.

EXAMPLE 2.7 Consider the initial value problem

$$\frac{dy}{dt} = -y^3, \quad \text{where} \quad y(0) \in \mathscr{R} \qquad (2.18)$$

Zero is the only fixed point of (2.18). Now suppose a numerical approximation is obtained using the Forward Euler method (2.9). This yields

$$y_{n+1} = y_n - hy_n^3 \qquad (2.19)$$

It is simple to check that $y_n = (-1)^n\sqrt{2/h}$ defines a period 2 solution of (2.19). Now suppose that the numerical solution is obtained using the method (2.20)

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 0{\cdot}5 & 0{\cdot}5 & 0 \\ \hline & 0{\cdot}5 & 0{\cdot}5 \end{array} \qquad (2.20)$$

One step of this method with step-size h corresponds to two steps of the Forward Euler method with step-size $h/2$. Thus for any $h > 0$ $y_n = \sqrt{4/h}$ and $y_n = -\sqrt{4/h}$ are both spurious fixed points of the method (2.20) for the problem (2.18).

Notice that the spurious solutions in the example exist for all h, but tend to infinity as $h \to 0$. We will later prove that if $\mathbf{f}$ is locally Lipschitz then 2-cycles of linear multistep methods which exist for arbitrarily small h tend to infinity as $h \to 0$. We would also like to prove this result for the spurious fixed points of Runge–Kutta methods, but the example below shows that it does not hold for these methods without further assumptions.

EXAMPLE 2.8 Consider the initial value problem

$$\frac{dy}{dt} = f_1(y) = y^3, \quad \text{where} \quad y(0) \in \mathfrak{R}. \tag{2.21}$$

Zero is the only fixed point of (2.21). Now suppose a numerical approximation is obtained using the Runge–Kutta method (2.22).

$$\begin{array}{c|cc} 1 & 0{\cdot}75 & 0{\cdot}25 \\ 1 & 0{\cdot}25 & 0{\cdot}75 \\ \hline & 0{\cdot}5 & 0{\cdot}5 \end{array} \tag{2.22}$$

Let $y_n = 0$, then it is simple to check that (2.23) solves the equations (2.1–2) for the method (2.22) and any $h > 0$ where $\mathbf{f}$ is given by f_1.

$$\begin{aligned} y_n &= y_{n+1} = 0 \\ Y_1 &= \sqrt{2/h} \\ Y_2 &= -\sqrt{2/h} \end{aligned} \tag{2.23}$$

Now consider the modified problem

$$\frac{dy}{dt} = f_2(y) = (y + p(y))^3, \quad \text{where} \quad y(0) \in \mathfrak{R} \tag{2.24}$$

and p is the test function

$$p(y) = \begin{cases} 0 & \text{if } |y| \geq 1 \\ \exp\,[1/(y^2 - 1)] & \text{if } |y| < 1. \end{cases}$$

Observe that $f_2(0) = e^{-3} \neq 0$, thus zero is not a fixed point of (2.24), also since p is a test function, (see [2]), $f_2 \in C^\infty(\mathfrak{R}, \mathfrak{R})$. Now consider the numerical solution using the Runge–Kutta method (2.22). For $|y| \geq 1$, $f_1(y) = f_2(y)$, therefore if $h \leq 2$ and $y_n = 0$ then (2.23) also solves the equations (2.1–2) for the modified problem (2.24). Thus we have a problem of the form (1.1), where $\mathbf{f}$ is smooth, and a Runge–Kutta method which generates a spurious fixed point which exists for h arbitrarily small and is itself fixed as $h \to 0$.

All hope is not lost however. It should be noted that in both the problems considered in Example 2.8 the equations (2.1) admit more than one solution. For f_1 the solution $y_n = y_{n+1} = Y_1 = Y_2 = 0$ is far more 'natural' than the solution given in the example. In practical implementations of implicit Runge–Kutta methods, the equations (2.1) are often solved using an iteration scheme. We claim that any 'sensible' iteration scheme will converge to the 'natural' solution of the equations, and the spurious fixed solution seen in the example will not arise in practice. Although results similar to those that follow could be proved for any 'sensible' iteration scheme, the technicalities of the proofs depend on the specific scheme used, and we will assume throughout the rest of this chapter that when the Runge–Kutta equations (2.1) are implicit then they are solved using the Butcher iteration (2.11).

We need to prove a number of preliminary results before we can justify our claim. First we prove the existence of a (not necessarily unique) solution of the equations (2.1–2) when the condition that $\mathbf{f}$ is globally Lipschitz is relaxed.

In the following proposition and many of the subsequent technical results in this paper we will require U_δ to be a subset of some set U, such that

$$\inf_{\mathbf{y}\in\Re^m\setminus U}\ \inf_{\mathbf{x}\in U_\delta} \|\mathbf{x}-\mathbf{y}\| \geq \delta. \tag{2.25}$$

This is equivalent to requiring the boundaries of U_δ and U to be separated by distance at least δ, (where the distance function is induced by the norm), so that for any $\mathbf{x} \in U_\delta$, the closed ball of radius δ about $\mathbf{x}$, $\bar{B}(\mathbf{x}, \delta)$, is contained in U.

PROPOSITION 2.9 Suppose $\mathbf{f}$ is continuous on a compact set U, and $U_\delta \subset U$ such that (2.25) holds, let

$$M = \sup_{\mathbf{y}\in U} \|\mathbf{f}(\mathbf{y})\| \tag{2.26}$$

and suppose

$$h < \frac{\delta}{aM}. \tag{2.27}$$

Then if $\mathbf{y}_n \in U_\delta$ there exists a solution of the equations (2.1–2) such that

$$\|\mathbf{Y}_i - \mathbf{y}_n\| < \delta \qquad \forall i \tag{2.28}$$

and thus $\mathbf{Y}_i \in U\ \forall i$. Furthermore, if the iteration (2.11) converges, then it converges to such a solution.

Proof. Consider the iteration (2.11). Denote the cartesian product of s closed balls $\bar{B}(\mathbf{y}_n, \delta)$, by $\bar{B}(\mathbf{y}_n, \delta)^s$. Now suppose

$$(\mathbf{Y}_1^N, \mathbf{Y}_2^N, \ldots, \mathbf{Y}_s^N) \in \bar{B}(\mathbf{y}_n, \delta)^s$$

Then (2.11) and (2.27) imply

$$(\mathbf{Y}_1^{N+1}, \mathbf{Y}_2^{N+1}, \ldots, \mathbf{Y}_s^{N+1}) \in B(\mathbf{y}_n, \delta)^s$$

Furthermore, since $\mathbf{f}$ is continuous on U the iteration (2.11) defines a continuous map from the convex compact set $\bar{B}(\mathbf{y}_n, \delta)^s$ into itself. Thus by Brouwer's Fixed Point Theorem [6] there exists a fixed point of the iteration (2.11) within $\bar{B}(\mathbf{y}_n, \delta)^s$. This defines the required solution of (2.1–2). □

NOTE. We have not proved any of the following:

(i) that there is a unique solution of (2.1–2) satisfying the conditions of Proposition 2.9,

(ii) that there is not a solution of (2.1–2) such that $\|\mathbf{Y}_i - \mathbf{y}_n\| > \delta$ for some (or all) i,

(iii) that the iteration (2.11) converges.

If we assume that $\mathbf{f}$ is Lipschitz on U then we can prove that (i) and (iii) hold.

PROPOSITION 2.10 If $\mathbf{f}$ is Lipschitz on bounded U, with $U_\delta \subset U$ such that (2.25) holds and if

$$h < \min\left(\frac{\delta}{aM}, \frac{1}{La}\right) \tag{2.29}$$

where M is defined by (2.26) and L is the Lipschitz constant, then for any $\mathbf{y}_n \in U_\delta$ there exists a solution of the equations (2.1–2), such that $\mathbf{Y}_i \in U\ \forall i$, furthermore there is a unique solution with this property and the iteration (2.11) converges to this solution.

Proof. By the proof of Proposition 2.9

$$\|\mathbf{Y}_j^N - \mathbf{y}_n\| \leqslant \delta \qquad \forall j, N.$$

So $\mathbf{Y}_j^N \in U\ \forall j, N$. Now $\mathbf{f}$ is Lipschitz on U and although Theorem 2.3 does not apply in this case, Butcher's proof [1] holds, to give the required result. □

In neither of the above cases is it proved that a solution sequence $\{\mathbf{y}_n\}_{n=0}^{\infty}$ can be generated using the iteration (2.11) with fixed step-size, but the aim of this paper is to study the existence of spurious solutions, so we will assume that a solution sequence exists, with the equations (2.1–2) being solved exactly, then Proposition 2.9 and Proposition 2.10 will enable us to derive results on the nature of the spurious solutions.

All the remaining results in this section will follow from the two lemmas below.

LEMMA 2.11 If $\mathbf{f}$ is Lipschitz on bounded U, with $U_\delta \subset U$ such that (2.25) holds and

$$h < \min\left(\frac{\delta}{aM}, \frac{1}{L\mathscr{A}(1+B)}\right)$$

where M is defined by (2.26) and L is the Lipschitz constant, then the solution of the equations (2.1–2) satisfies $\mathbf{y}_n = \mathbf{y}_{n+1}$ with $\mathbf{y}_n \in U_\delta$ if and only if $\mathbf{f}(\mathbf{y}_n) = 0$; where we assume that if the method is implicit, then (2.1) is solved using the iteration (2.11).

Proof. Proposition 2.10 implies that the conditions for Lemma 2.4 hold and hence (2.13) holds. Now suppose that there exists a solution of (2.1–2) such that $\mathbf{y}_n = \mathbf{y}_{n+1}$ with $\mathbf{f}(\mathbf{y}_n) \neq 0$ and $\mathbf{y}_n \in U_\delta$, and follow the proof of Theorem 2.5 from (2.16) to obtain the result. □

LEMMA 2.12 Suppose $\mathbf{f}$ is continuous on a compact set U, and that if the Runge–Kutta method is implicit, then (2.1) is solved using the iteration (2.11), then given any $U_\delta \subset U$ such that (2.25) holds and any $\varepsilon > 0$ there exists $H(\varepsilon) > 0$ such that for $h < H(\varepsilon)$ any fixed solution $\hat{\mathbf{y}}$ of (2.1–2) such that $\hat{\mathbf{y}} \in U_\delta$ satisfies $\|\mathbf{f}(\hat{\mathbf{y}})\| < \varepsilon$.

Proof. Since U is compact, $\mathbf{f}$ is uniformly continuous on U, so given $\varepsilon_1 > 0\ \exists \delta_1 > 0$ such that for any $\mathbf{x}, \mathbf{y} \in U$ satisfying $\|\mathbf{x} - \mathbf{y}\| < \delta_1$ then $\|\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{y})\| < \varepsilon_1$. Let $\varepsilon_1 = \varepsilon/B$, $\delta_2 = \min(\delta, \delta_1)$ and $U_{\delta_2} = \{\mathbf{x} \in \mathscr{R}^m : \inf_{\mathbf{y} \in \mathscr{R}^m \setminus U} \|\mathbf{x} - \mathbf{y}\| \geqslant \delta_2\}$. By Proposition 2.9 if $h < (\delta_2/aM)$ then for any $\mathbf{y}_n \in U_{\delta_2}$ it follows that $\|\mathbf{Y}_i - \mathbf{y}_n\| < \delta_2$. Hence if $\mathbf{y}_n$ is a fixed point solution of (2.1–2) it follows that;

$$\begin{aligned} \|\mathbf{f}(\mathbf{y}_n)\| &= \left\|\sum_{i=1}^{s} b_i \mathbf{f}(\mathbf{y}_n)\right\| \\ &= \left\|\sum_{i=1}^{s} b_i(\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{Y}_i))\right\| \\ &< B\varepsilon_1 \\ &= \varepsilon \end{aligned}$$

and the result follows since $U_\delta \subseteq U_{\delta_2}$. □

Example 2.7 showed that it is possible for spurious solutions to exist for h arbitrarily small when f is locally Lipschitz, and we can now prove that such spurious solutions tend to infinity as $h \to 0$.

THEOREM 2.13 Suppose $\mathbf{f}$ is locally Lipschitz, and that if the method is implicit, (2.1) is solved using the iteration (2.11), then if spurious fixed point solutions of (2.1–2) exist for h arbitrarily small then these tend to infinity in norm as $h \to 0$. By this we mean that if there exists a sequence $(\mathbf{u}_p, h_p)$ such that $h_p > 0\ \forall p$, $h_p \to 0$ as $p \to \infty$ and $\mathbf{u}_p$ is a spurious fixed point of the method with step-size h_p then $\|\mathbf{u}_p\| \to \infty$ as $p \to \infty$.

Proof. It is sufficient to prove that for any bounded set D, for h sufficiently small no point of D is a spurious fixed point. Since D is bounded, for some $r > 0$, $D \subset \bar{B}(0, r)$, where $\bar{B}(0, r)$ is the closed ball of radius r centred at the origin. Let $U_\delta = \bar{B}(0, r)$ and $U = \bar{B}(0, r + 1)$. Fix $\delta = 1$, then the result follows from Lemma 2.11. □

COROLLARY 2.14 Suppose $\mathbf{f} \in C^1(\mathcal{R}^m, \mathcal{R}^m)$, and that, if the method is implicit, the equations (2.1–2) are solved using the iteration (2.11), then if spurious fixed point solutions exist for h arbitrarily small then these tend to infinity in norm as $h \to 0$.

An alternative statement of Theorem 2.13 is to say that if a continuous branch (or bounded sequence) of fixed point solutions exists as $h \to 0$ then $\exists H > 0$ such that for $h < H$ the corresponding fixed point solution of (2.1–2), $\mathbf{u}$, satisfies $\mathbf{f}(\mathbf{u}) = 0$, that is $\mathbf{u}$ is a fixed point solution of (1.1). If we relax the condition that $\mathbf{f}$ is Lipschitz continuous and assume merely that $\mathbf{f}$ is continuous on $\mathcal{R}^m$ then the following theorem shows that continuous branches of spurious fixed point solutions which exist for h arbitrarily small, either tend to steady solutions of the underlying differential equation, or diverge to infinity as $h \to 0$.

THEOREM 2.15 Suppose $\mathbf{f}$ is continuous on $\mathcal{R}^m$ and there exists a continuous branch of fixed points $\mathbf{u}(h)$ of (2.1–2) for $h \in (0, H]$, where for an implicit method (2.1) is solved using the iteration (2.11), then as $h \to 0$ either

(i) $\|\mathbf{f}(\mathbf{u}(h))\| \to 0$, or,
(ii) $\|\mathbf{u}(h)\| \to \infty$.

If furthermore the zeros of $\mathbf{f}$ are isolated then (i) implies that $\mathbf{u}(h) \to \tilde{\mathbf{y}}$, a steady solution of (1.1), as $h \to 0$.

Proof. It is sufficient to show that as $h \to 0$, for any compact D, $\|\mathbf{f}(\mathbf{u}(h))\| \to 0$ or for all sufficiently small h, $\mathbf{u}(h)$ is not in D. Let $U_\delta = D$. Fix $\delta = 1$. Let $U = \{\mathbf{x} \in \mathcal{R}^m : \inf_{\mathbf{y} \in U_\delta} \|\mathbf{x} - \mathbf{y}\| \leq \delta\}$ then apply Lemma 2.12. If the zeros of $\mathbf{f}$ are isolated then the last part follows by the continuity of $\mathbf{f}$. □

NOTE. Example 3.6 shows that if $\mathbf{f}$ is continuous on $\mathcal{R}^m$ it is possible for a Runge–Kutta method to generate a spurious fixed point solution which remains bounded and which converges to a steady solution of (1.1) as $h \to 0$.

The following theorem gives a necessary condition for the bifurcation of spurious fixed solutions from $\tilde{\mathbf{y}}$ at $h = 0$, namely either

(a) $\mathbf{f}$ is not continuous at $\tilde{\mathbf{y}}$, or,
(b) $\mathbf{f}(\tilde{\mathbf{y}}) = 0$ and $\mathbf{f}$ is not Lipschitz at $\tilde{\mathbf{y}}$.

THEOREM 2.16 Suppose there exists a sequence $(\mathbf{u}_p, h_p)$ such that $h_p > 0\ \forall p$, $h_p \to 0$, and $\mathbf{u}_p \to \tilde{\mathbf{y}}$ as $p \to \infty$ where, for each p, $\mathbf{u}_p$ is a spurious fixed point solution of (2.1–2) with step-size h_p, and if the method is implicit (2.1) is solved using the iteration scheme (2.11), then if $\mathbf{f}$ is continuous on a neighbourhood of $\tilde{\mathbf{y}}$ it follows that

(i) $\mathbf{f}(\tilde{\mathbf{y}}) = 0$, that is $\tilde{\mathbf{y}}$ is a steady solution of (1.1).
(ii) $\mathbf{f}$ is not Lipschitz at $\tilde{\mathbf{y}}$.

Proof. (i) By Lemma 2.12 $\|\mathbf{f}(\mathbf{u}_p)\| \to 0$ as $p \to \infty$, and result follows by continuity of $\mathbf{f}$. (ii) Follows trivially from Lemma 2.11. □

NOTE. The above theorem also shows that if the numerical method is asymptotic to $\tilde{\mathbf{y}}$ for arbitrarily small h then $\tilde{\mathbf{y}}$ is a genuine asymptotic fixed point of (1.1), (although it does not necessarily follow that the solution of the continuous problem is asymptotic to $\tilde{\mathbf{y}}$ if the same initial value is used as for the numerical method).

Now consider general $\mathbf{f}$ but suppose $\mathbf{f}$ is Lipschitz on an open set U. Notice that by Lemma 2.11 if $\tilde{\mathbf{y}} \in U$ is a spurious fixed point solution and $h < H(\delta)$ then $\tilde{\mathbf{y}}$ is within distance δ of ∂U. We can force spurious fixed points to ∂U by taking δ as small as we like. By (2.27) as $\delta \to 0$, $H(\delta) \to 0$. In this way we prove that as $h \to 0$ spurious fixed points either 'converge' to the set on which $\mathbf{f}$ is not Lipschitz or 'diverge' to infinity.

COROLLARY 2.17 Suppose $\mathbf{f}$ is Lipschitz on every bounded subset of some set D, and if the method is implicit (2.1) is solved using the iteration scheme (2.11), then given any positive δ, β there exists $H(\delta, \beta) > 0$ such that every spurious fixed point $\tilde{\mathbf{y}}$ of (2.1–2) with $h < H(\delta, \beta)$, satisfies either

(i) $\inf_{x \notin D} \|\tilde{\mathbf{y}} - \mathbf{x}\| < \delta$,

or

(ii) $\|\tilde{\mathbf{y}}\| > \beta$.

Proof. Take $U = \bar{B}(0, \beta + \delta) \cap D$ and $U_\delta = \{\mathbf{x} \in U : \inf_{\mathbf{y} \in \mathcal{R}^m \setminus U} \|\mathbf{x} - \mathbf{y}\| \geq \delta\}$ and apply Lemma 2.11. □

If the Lipschitz condition is dropped the following result holds.

COROLLARY 2.18 Suppose $\mathbf{f}$ is continuous on every bounded subset of some set D, and if the method is implicit (2.1) is solved using the iterations scheme (2.11), then given any positive ε, β, δ there exists $H(\varepsilon, \beta, \delta) > 0$ such that every spurious fixed point $\bar{\mathbf{y}}$ of (2.1–2) with $h < H(\varepsilon, \beta, \delta)$, satisfies either

(i) $\inf_{x \notin D} \|\bar{\mathbf{y}} - \mathbf{x}\| < \delta$,

or

(ii) $\|\bar{\mathbf{y}}\| > \beta$.

or

(iii) $\|\mathbf{f}(\bar{\mathbf{y}})\| < \varepsilon$,

Proof. With U and U_δ defined as in the proof of Corollary 2.17 apply Lemma 2.12. □

3. Spurious period two solutions of Runge–Kutta methods

In this section we will prove results for (spurious) period 2 solutions of Runge–Kutta methods analogous to those proved in the last section for spurious fixed points of these methods. Recall that a period 2 solution of (2.1–2) is a solution sequence of the form $\mathbf{y}_{2n} = \mathbf{u}$, $\mathbf{y}_{2n+1} = \mathbf{v}$ where $\mathbf{u} \neq \mathbf{v}$. We begin by showing that 2-cycles cannot exist for h arbitrarily small if $\mathbf{f}$ is globally Lipschitz. This result follows as a simple corollary of Theorem 2.5.

THEOREM 3.1 If $\mathbf{f}$ is globally Lipschitz, with Lipschitz constant L, and

$$h < \frac{1}{L(1+\mathscr{A})(1+B)} \tag{3.1}$$

then the Runge–Kutta method (2.1–2) admits no period 2 solutions when applied to (1.1).

Proof. Following Iserles *et al.* [8] define the inflated method corresponding to the Runge–Kutta scheme (2.1–2) by

$$\begin{array}{c|cc} \frac{1}{2}\mathbf{c} & \frac{1}{2}A & 0 \\ \frac{1}{2}\mathbf{1} + \frac{1}{2}\mathbf{c} & \frac{1}{2}D & \frac{1}{2}A \\ \hline & \frac{1}{2}\mathbf{b}^T & \frac{1}{2}\mathbf{b}^T \end{array} \tag{3.2}$$

where A, $\mathbf{b}^T$ and $\mathbf{c}$ are defined by (2.3) and

$$D = \begin{bmatrix} \mathbf{b}^T \\ \vdots \\ \mathbf{b}^T \end{bmatrix}.$$

Note that two steps of the original method with step-size h corresponds to one step of the inflated method with step-size $2h$. Thus a period 2 solution of (2.1–2) with step-size h corresponds to a fixed point of (3.2) with step-size $2h$. By Theorem 2.5 the inflated method admits no spurious fixed points if

$$h < \frac{2}{L(1+\mathscr{A})(1+B)}$$

and therefore if $(\mathbf{u}, \mathbf{v})$ is a 2-cycle of (2.1–2) where h satisfies (3.1) then $\mathbf{u}, \mathbf{v}$ are both fixed points of (1.1). Trivially then $\mathbf{u}, \mathbf{v}$ are both fixed points of (2.1–2), but by Theorem 2.3, the solution of (2.1–2) is unique, hence $\mathbf{u} = \mathbf{v}$, therefore no such 2-cycle exists. □

We can apply the other results of the previous section to the inflated method to derive the equivalent results for the 2-cycles of explicit Runge–Kutta methods, but we are not able to derive satisfactory results for implicit methods using this technique. This is because the results in Section 2 are iteration dependent, and although we can use these results to prove that the inflated method has no spurious fixed points (and hence the Runge–Kutta method admits no period 2 solutions), the new results will only hold if the iteration scheme used to solve (2.1–2) is equivalent to solving the inflated method by (2.11). This means we must solve for *two* steps of (2.1–2) simultaneously, not a scheme used in practice. Instead we will prove these results directly in the case where (2.1–2) is solved using (2.11). First we set up some notation.

Suppose $\mathbf{y}_{2n} = \mathbf{u}$, $\mathbf{y}_{2n+1} = \mathbf{v}$ with $\mathbf{u} \neq \mathbf{v}$ is a period two solution of the Runge–Kutta method (2.1–2). Then writing $\mathbf{U}_i$ for the internal stage values at the $(2n)$th step, and $\mathbf{V}_i$ for the stage values at the $(2n+1)$th step, it follows that:

$$\mathbf{u} = \mathbf{v} + h \sum_{i=1}^{s} b_i \mathbf{f}(\mathbf{U}_i) \tag{3.3}$$

$$\mathbf{U}_i = \mathbf{v} + h \sum_{j=1}^{s} a_{ij} \mathbf{f}(\mathbf{U}_j) \tag{3.4}$$

$$\mathbf{v} = \mathbf{u} + h \sum_{i=1}^{s} b_i \mathbf{f}(\mathbf{V}_i) \tag{3.5}$$

$$\mathbf{V}_i = \mathbf{u} + h \sum_{j=1}^{s} a_{ij} \mathbf{f}(\mathbf{V}_j). \tag{3.6}$$

Adding (3.3) and (3.5) implies

$$\sum_{i=1}^{s} b_i [\mathbf{f}(\mathbf{U}_i) + \mathbf{f}(\mathbf{V}_i)] = 0 \tag{3.7}$$

The following Lemma provides a bound on the solution, when a Lipschitz condition is assumed, which is complementary to Lemma 2.4 and together these two lemmas will enable us to prove directly that 2-cycles cannot exist in certain regions for h arbitrarily small if $\mathbf{f}$ satisfies a Lipschitz condition.

Lemma 3.2 If $\mathbf{f}$ is Lipschitz on U with Lipschitz constant L, $\mathbf{Y}_n \in U$ and $\mathbf{Y}_i \in U\ \forall i$ and

$$h < \frac{1}{L(\mathscr{A} + B)} \tag{3.8}$$

then the numerical solution defined by (2.1–2) satisfies

$$\|\mathbf{f}(\mathbf{y}_{n+1}) - \mathbf{f}(\mathbf{Y}_i)\| < \frac{Lh(\mathscr{A} + B)}{1 - Lh(\mathscr{A} + B)} \|\mathbf{f}(\mathbf{y}_{n+1})\| \qquad \forall i = 1, \ldots, s \tag{3.9}$$

Proof. With the notation of the proof of Lemma 2.4 observe

$$\begin{aligned}\|\mathbf{f}(\mathbf{y}_{n+1})-\mathbf{f}(\mathbf{Y}_i)\| &= \left\|\mathbf{f}\left(\mathbf{y}_n + h\sum_{j=1}^{s} b_j\mathbf{f}(\mathbf{Y}_j)\right)-\mathbf{f}\left(\mathbf{y}_n + h\sum_{j=1}^{s} a_{i,j}\mathbf{f}(\mathbf{Y}_j)\right)\right\| \\ &\leq Lh\left\|\sum_{j=1}^{s} b_j\mathbf{f}(\mathbf{Y}_j)-\sum_{j=1}^{s} a_{i,j}\mathbf{f}(\mathbf{Y}_j)\right\| \\ &\leq Lh(\mathscr{A}+B)M\end{aligned}$$

The remainder of the proof is similar to that of Lemma 2.4. □

Now we prove results equivalent to Proposition 2.9 and Proposition 2.10; and from which all the remaining results in this section follow.

PROPOSITION 3.3 If $\mathbf{f}$ is Lipschitz on bounded U, with $U_\delta \subset U$ such that (2.25) holds then there exists $H(\delta)>0$ such that no point of U_δ is contained in a 2-cycle of the method (2.1–2) with step-size $h<H(\delta)$, where (2.1) is solved using the iteration (2.11), if the method is implicit.

Proof. Let $U_{\delta/2}=\{\mathbf{x}:\inf_{\mathbf{y}\in U_\delta}\|\mathbf{x}-\mathbf{y}\|\leq\delta/2\}$. By Proposition 2.10 $\exists H(\delta)>0$ such that for any $\mathbf{y}_n\in U_\delta$, the solution of (2.1–2) is such that $\mathbf{Y}_i\in U_{\delta/2}$. Reducing $H(\delta)$ if necessary to ensure $h<(\delta/4BM)$ where $M=\sup_{\mathbf{y}\in U}\|\mathbf{f}(\mathbf{y})\|$ then we also have $\mathbf{y}_{n+1}\in U_{\delta/2}$. Then similarly at the next step $\mathbf{y}_{n+2}$ and the associated stage values are contained in U. Now suppose $(\mathbf{u},\mathbf{v})$ is a 2-cycle with $\mathbf{u}\in U_\delta$, then $\mathbf{v}\in U_{\delta/2}$. Again reducing $H(\delta)$ if necessary so that $h<[1/L(\mathscr{A}+B)]$, where L is the Lipschitz constant, Lemmas 2.4 and 3.2 apply, so we have;

$$\|\mathbf{f}(\mathbf{u})-\mathbf{f}(\mathbf{U}_i)\|<\frac{Lh(\mathscr{A}+B)}{1-Lh(\mathscr{A}+B)}\|\mathbf{f}(\mathbf{u})\| \qquad \forall i=1,\ldots,s$$

$$\|\mathbf{f}(\mathbf{u})-\mathbf{f}(\mathbf{V}_i)\|<\frac{L\mathscr{A}h}{1-L\mathscr{A}h}\|\mathbf{f}(\mathbf{u})\| \qquad \forall i=1,\ldots,s$$

Then

$$\begin{aligned}\left\|\sum_{i=1}^{s} b_i[\mathbf{f}(\mathbf{U}_i)+\mathbf{f}(\mathbf{V}_i)]\right\| &> \|\mathbf{f}(\mathbf{u})\|\left[2-\frac{Lh\mathscr{A}B}{1-Lh\mathscr{A}}-\frac{Lh(\mathscr{A}+B)B}{1-Lh(\mathscr{A}+B)}\right] \\ &= \|\mathbf{f}(\mathbf{u})\|\left[\frac{2-hL(B+2)(B+2\mathscr{A})+2h^2L^2\mathscr{A}(\mathscr{A}+B)(1+B)}{(1-hL\mathscr{A})(1-hL(\mathscr{A}+B))}\right]\end{aligned}$$

Again reducing $H(\delta)$ if necessary we can assume $\|\mathbf{f}(\mathbf{u})\|>0$ otherwise, $\mathbf{u}$ is a fixed point of (1.1), which must solve (2.1–2), but since $\mathbf{u}\neq\mathbf{v}$ this implies that the solution of (2.1–2) is not unique in U, contradicting Proposition 2.10. Thus $h<2/L(B+2)(B+2\mathscr{A})$ implies

$$\left\|\sum_{i=1}^{s} b_i[\mathbf{f}(\mathbf{U}_i)+\mathbf{f}(\mathbf{V}_i)]\right\|>0$$

which contradicts (3.7). Therefore no point of U_δ is contained in a 2-cycle. □

PROPOSITION 3.4 Suppose $\mathbf{f}$ is continuous on compact U. Wtih $U_\delta \subset U$ such that (2.25) holds, then given $\varepsilon, \beta > 0$ there exists $H(\varepsilon, \beta) > 0$ such that if $\mathbf{u} \in U_\delta$ and $(\mathbf{u}, \mathbf{v})$ is a period 2 solution of (2.1–2) with $h < H(\varepsilon, \beta)$ then

(i) $\max(\|\mathbf{f}(\mathbf{u})\|, \|\mathbf{f}(\mathbf{v})\|) < \varepsilon$

(ii) $\|\mathbf{u} - \mathbf{v}\| < \beta$.

Proof. U compact implies $\mathbf{f}$ is uniformly continuous on U. Thus given $\varepsilon > 0\, \exists \delta_1 > 0$ such that for any $\mathbf{x}, \mathbf{y} \in U$ satisfying $\|\mathbf{x} - \mathbf{y}\| < \delta_1$ it follows that $\|\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{y})\| < \varepsilon$. Let $\delta_2 = \min(\delta, \delta_1, \beta)$. Define U_{δ_2} and $U_{(\delta_2/2)}$ to be the maximal sets consistent with (2.25). Let $M = \sup_{\mathbf{y} \in U} \|\mathbf{f}(\mathbf{y})\|$, and $H(\varepsilon, \beta) = \min[(\delta_2/2aM), (\delta_2/2BM)]$. By Proposition 2.9 for any $\mathbf{y}_n \in U_{\delta_2}$ if $h < H(\varepsilon, \beta)$ the solution of (2.1–2) satisfies $\|\mathbf{Y}_i - \mathbf{y}_n\| < (\delta_2/2)$, and furthermore, since $h < (\delta_2/2BM)$;

$$\|\mathbf{y}_{n+1} - \mathbf{y}_n\| < \frac{\delta_2}{2} < \beta, \tag{3.10}$$

that is $\mathbf{Y}_i \in U_{(\delta_2/2)}$ and $\mathbf{y}_{n+1} \in U_{(\delta_2/2)}$. Similarly at the next step $\mathbf{y}_{n+2}$ and the associated stage values are contained in U.

Now suppose $\mathbf{u} \in U_{\delta_2}$ and $(\mathbf{u}, \mathbf{v})$ is a two-cycle. Then by (3.10) and uniform continuity

$$\|\mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v})\| < \varepsilon$$

Also

$$\begin{aligned}
\|\mathbf{f}(\mathbf{u}) + \mathbf{f}(\mathbf{v})\| &= \left\|\sum_{i=1}^{s} b_i(\mathbf{f}(\mathbf{u}) + \mathbf{f}(\mathbf{v}))\right\| \\
&= \left\|\sum_{i=1}^{s} b_i(\mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{V}_i)) + \sum_{i=1}^{s} b_i(\mathbf{f}(\mathbf{v}) - \mathbf{f}(\mathbf{U}_i))\right\| \quad \text{by (3.7)} \\
&< 2B\varepsilon
\end{aligned}$$

and by the triangle inequality

$$\max(\|\mathbf{f}(\mathbf{u})\|, \|\mathbf{f}(\mathbf{v})\|) < \left(\frac{2B+1}{2}\right)\varepsilon. \tag{3.11}$$

Now the result follows on rescaling ε from (3.10) and (3.11), since $U_\delta \subseteq U_{\delta_2}$. □

The results below all follow from the propositions above, in a similar way to that in which the equivalent results were derived in the last Section. The proofs are omitted.

THEOREM 3.5 Suppose $\mathbf{f}$ is locally Lipschitz (in particular if $\mathbf{f} \in C^1(\mathcal{R}^m, \mathcal{R}^m)$), and that if the method is implicit, (2.1) is solved using the iteration (2.11), then if spurious period 2 solutions of (2.1–2) exist for h arbitrarily small then these tend to infinity in norm as $h \to 0$. By this we mean that if there exists a sequence $(\mathbf{u}_p, \mathbf{v}_p, h_p)$ such that $h_p > 0\, \forall p$, $h_p \to 0$ as $p \to \infty$ and $(\mathbf{u}_p, \mathbf{v}_p)$ is a period 2 solution of the method with step-size h_p then $\|\mathbf{u}_p\|, \|\mathbf{v}_p\| \to \infty$ as $p \to \infty$. □

If we relax the condition that $\mathbf{f}$ is locally Lipschitz continuous and assume merely that $\mathbf{f}$ is continuous on $\mathscr{R}^m$ then the following example shows that bounded spurious solutions can exist for h arbitrarily small.

EXAMPLE 3.6 Consider the initial value problem

$$\frac{dy}{dt}=f(y), \quad \text{where} \quad y(0)\in\mathscr{R} \tag{3.12}$$

where $f\in C(\mathscr{R}^m, \mathscr{R}^m)$ is defined by

$$f(y)=\begin{cases}-y^{\frac{1}{2}} & \text{if } y\geq 0\\ (-y)^{\frac{1}{2}} & \text{if } y\leq 0.\end{cases}$$

Zero is the only fixed point of (3.12). Now suppose a numerical approximation is obtained using the Forward Euler method (2.9). This yields

$$y_{n+1}=y_n+hf(y_n) \tag{3.13}$$

It is simple to check that $y_n=(-1)^n h^2/4$ defines a period 2 solution of (3.13) for any $h>0$. Now suppose that the numerical solution is obtained using the inflated method (2.20). One step of this method with step-size h corresponds to two steps of the Forward Euler method with step-size $h/2$. Thus for any $h>0$ $y_n=h^2/16$ and $y_n=-h^2/16$ are both spurious fixed points of the method (2.20) for the problem (3.12). Notice that all the spurious solutions in this example remain bounded as $h\to 0$, and furthermore they converge to steady solutions of (3.12).

The following theorem shows that if $\mathbf{f}$ is continuous on $\mathscr{R}^m$, then continuous branches of spurious period 2 solutions which exist for h arbitrarily small, either tend to steady solutions of the underlying differential equation, or diverge to infinity as $h\to 0$.

THEOREM 3.7 Suppose $\mathbf{f}$ is continuous on $\mathscr{R}^m$ and there exists a continuous branch of period 2 solutions $(\mathbf{u}(h), \mathbf{v}(h))$ of (2.1–2) for $h\in(0, H]$, where for an implicit method (2.1) is solved using the iteration (2.11). Then, as $h\to 0$, either

(i) $\|\mathbf{f}(\mathbf{u}(h))\|$, $\|\mathbf{f}(\mathbf{v}(h))\|$ and $\|\mathbf{u}(h)-\mathbf{v}(h)\|\to 0$, or,
(ii) $\|\mathbf{u}(h)\|$ and $\|\mathbf{v}(h)\|\to\infty$.

If furthermore the zeros of $\mathbf{f}$ are isolated then (i) implies that $\mathbf{u}(h), \mathbf{v}(h)\to\bar{\mathbf{y}}$, a steady solution of (1.1), as $h\to 0$. □

The following theorem gives the same necessary condition for the bifurcation of period 2 solutions from $\bar{\mathbf{y}}$ at $h=0$, as was found for spurious fixed points, namely either

(a) $\mathbf{f}$ is not continuous at $\bar{\mathbf{y}}$, or,
(b) $\mathbf{f}(\bar{\mathbf{y}})=0$ and $\mathbf{f}$ is not Lipschitz at $\bar{\mathbf{y}}$.

THEOREM 3.8 Suppose there exists a sequence $(\mathbf{u}_p, \mathbf{v}_p, h_p)$ such that $h_p>0\,\forall p$, $h_p\to 0$, $\mathbf{u}_p\to\bar{\mathbf{y}}$ as $p\to\infty$ and $(\mathbf{u}_p, \mathbf{v}_p)$ is a period 2 solution of (2.1–2) with step-size h_p for all p, where for an implicit method (2.1) is solved using the iteration (2.11), and $\mathbf{f}$ is continuous on a neighbourhood of $\tilde{\mathbf{y}}$. Then

(i) $\mathbf{v}_p \to \tilde{\mathbf{y}}$ as $p \to \infty$

(ii) $\mathbf{f}(\tilde{\mathbf{y}}) = 0$, that is $\tilde{\mathbf{y}}$ is a fixed point of (1.1).

(iii) $\mathbf{f}$ is not Lipschitz at $\tilde{\mathbf{y}}$. □

COROLLARY 3.9 Suppose $\mathbf{f}$ is Lipschitz on every bounded subset of some set D, and if the method is implicit (2.1) is solved using the iteration (2.11), then given any positive δ, β there exists $H(\delta, \beta) > 0$ such that every point $\mathbf{u}$ contained in a 2-cycle of (2.1–2) with $h < H(\delta, \beta)$, satisfies either

(i) $\inf_{x \notin D} \|\mathbf{u} - \mathbf{x}\| < \delta$,

or

(ii) $\|\mathbf{u}\| > \beta$. □

COROLLARY 3.10 Suppose $\mathbf{f}$ is continuous on every bounded subset of some set D, and if the method is implicit (2.1) is solved using the iteration (2.11), then given any positive ε, β, δ there exists $H(\varepsilon, \beta, \delta) > 0$ such that every point $\mathbf{u}$ contained in a 2-cycle of (2.1–2) with $h < H(\varepsilon, \beta, \delta)$ satisfies either

(i) $\inf_{x \notin D} \|\mathbf{u} - \mathbf{x}\| < \delta$,

or

(ii) $\|\mathbf{u}\| > \beta$.

or

(iii) $\|\mathbf{f}(\mathbf{u})\|, \|\mathbf{f}(\mathbf{v})\| < \varepsilon$, and $\|\mathbf{u} - \mathbf{v}\| < \delta$, where $\mathbf{v}$ is the other point of the 2-cycle. □

4. Spurious period two solutions of linear multistep methods

Consider approximating the solution of (1.1) using a general consistent k-step linear multistep method

$$\sum_{j=0}^{k} \alpha_j \mathbf{Y}_{n+j} = h \sum_{j=0}^{k} \beta_j \mathbf{f}(\mathbf{Y}_{n+j}) \tag{4.1}$$

with fixed step-size $h > 0$. $\mathbf{Y}_n$ approximates the exact solution of (1.1) at $t = nh$, and it is assumed the starting values $\mathbf{Y}_0, \ldots, \mathbf{Y}_{k-1}$ are given. Define the polynomials $\rho(z)$, $\sigma(z)$ by

$$\rho(z) = \sum_{j=0}^{k} \alpha_j z^j, \qquad \sigma(z) = \sum_{j=0}^{k} \beta_j z^j. \tag{4.2}$$

Without loss of generality assume $\alpha_k = 1$. We will assume throughout that the method (4.1) is consistent. This implies that

$$\rho(1) = 0, \qquad \sigma(1) = \rho'(1) = b. \tag{4.3}$$

For a zero-stable method b is a nonzero constant. If $\beta_k \neq 0$ then the method is implicit. The dynamics of these methods has been studied extensively. In particular:

THEOREM 4.1 (Iserles [7]) For a zero-stable linear multistep method (4.1), $\hat{\mathbf{Y}}$ is a fixed point if and only if $\mathbf{f}(\hat{\mathbf{Y}}) = 0$.

Thus the method is $R^{[1]}$ and hence preserves all fixed asymptotic points of (1.1), and furthermore introduces no spurious steady solutions. However as with all previous methods which are $R^{[1]}$ it does not necessarily follow that the solution of the continuous problem is asymptotic to the same point as the numerical method even when the same initial value is used. No $R^{[1]}$ Runge–Kutta methods are known with order >4 whereas we can obtain linear multistep methods of arbitrarily high order, hence these methods would seem to be very good for the long term simulation of systems (1.1) which are convergent to steady solutions as $T \to \infty$. The linear multistep methods which do not admit period 2 solutions have been studied in [8, 9, 12]. The following example shows that period 2 solutions can be constructed trivially if $\rho(-1) = 0$.

EXAMPLE 4.2 (Iserles, Peplow and Stuart [8]) If $\rho(-1) = 0$ then take any $\mathbf{f}$ which has at least two fixed points. If $\mathbf{f}(\bar{\mathbf{y}}) = \mathbf{f}(\hat{\mathbf{y}}) = 0$ with $\hat{\mathbf{y}} \neq \bar{\mathbf{y}}$ then it is easy to check that

$$\mathbf{Y}_n = \left(\frac{\bar{\mathbf{y}} + \hat{\mathbf{y}}}{2}\right) + \left(\frac{\bar{\mathbf{y}} - \hat{\mathbf{y}}}{2}\right)(-1)^n \tag{4.4}$$

is a period 2 solution which satisfies (4.1), for any $h > 0$.

The above example prevents us from extending the results of the previous section to cover all zero-stable linear multistep methods, since the 2-cycles of Example 4.2 exist independently of the step-size h. However if we exclude the case $\rho(-1) = 0$ we may proceed to prove similar results for period 2 solutions of linear multistep methods as we prove for Runge–Kutta methods. The following lemma, which shows that if the step-size is fixed then there is at most one 2-cycle passing through any point of the space, provides the key to this approach.

LEMMA 4.3 Suppose the linear multistep method (4.1) is zero-stable with $\rho(-1) \neq 0$, then a 2-cycle $(\mathbf{u}, \mathbf{v})$ of the method with step-size h satisfies $\mathbf{f}(\mathbf{u}) \neq 0$, $\mathbf{f}(\mathbf{v}) \neq 0$,

$$\mathbf{f}(\mathbf{u}) + \mathbf{f}(\mathbf{v}) = 0 \tag{4.5}$$

and

$$\mathbf{u} = \mathbf{v} - \frac{2h\sigma(-1)\mathbf{f}(\mathbf{v})}{\rho(-1)}. \tag{4.6}$$

Proof. In Section 2 of [9] it is shown that a 2-cycle of a linear multistep method satisfies

$$h\sigma(1)[\mathbf{f}(\mathbf{u}) + \mathbf{f}(\mathbf{v})] = 0 \tag{4.7}$$

and

$$h\sigma(-1)[\mathbf{f}(\mathbf{v}) - \mathbf{f}(\mathbf{u})] = \rho(-1)[\mathbf{v} - \mathbf{u}]. \tag{4.8}$$

Since the method is zero-stable (4.5) follows from (4.7). Hence (4.8) simplifies to

$$\rho(-1)[\mathbf{v} - \mathbf{u}] = 2h\sigma(-1)\mathbf{f}(\mathbf{v}),$$

and rearranging gives (4.6). Finally if $\mathbf{f}(\mathbf{u}) = 0$ or $\mathbf{f}(\mathbf{v}) = 0$ then (4.5–6) imply that $\mathbf{u} = \mathbf{v}$, a contradiction since $(\mathbf{u}, \mathbf{v})$ form a 2-cycle. □

Lemma 4.3 allows us to classify explicitly the linear multistep methods which do not admit period 2 solutions.

THEOREM 4.4
(i) The linear multistep method (4.1) is not $R^{[2]}$ if $\rho(-1) = 0$.
(ii) If $\rho(-1) \neq 0$ and the method (4.1) is zero-stable then it is $R^{[2]}$ if and only if $\sigma(-1) = 0$.

NOTE. Theorem 4.4 is a slight generalization of a result of Iserles *et al.* [8], who proved the classification in (ii) for irreducible methods. The result of Iserles *et al.* was itself a generalization of an earlier result of Stuart and Peplow [12].

Proof. (i) See Example 4.2.
(ii) The 'if' part follows from (4.6), since if $\sigma(-1) = 0$ then $\mathbf{u} = \mathbf{v}$ which contradicts that $(\mathbf{u}, \mathbf{v})$ form a 2-cycle. To prove the 'only if' part, take any $\mathbf{f} \in C(\mathcal{R}, \mathcal{R})$ such that $\mathbf{f}(0) = -1$ and $\mathbf{f}(2h\sigma(-1)/\rho(-1)) = 1$. Let $\mathbf{v} = 0$ and $\mathbf{u} = (2h\sigma(-1))/\rho(-1)$, then it is simple to check that $(\mathbf{u}, \mathbf{v})$ form a 2-cycle. □

Thus the class of zero-stable linear multistep methods which satisfy $\rho(-1) \neq 0$ and $\sigma(-1) = 0$ is $R^{[1,2]}$, and by considering this class of methods we can generate methods of arbitrarily high order which are $R^{[1,2]}$.

Lemma 4.3 also allows us to prove the following two propositions for linear multistep methods equivalent to Propositions 3.3 and 3.4 for Runge–Kutta methods. Note that whilst the Runge–Kutta results only hold if the equations (2.1–2) are solved exactly via the iteration (2.11) the following results hold whenever (4.1) is solved exactly, independently of the method which is used to find this solution. Thus in this section we do not need to make any assumption about the scheme used to solve (4.1).

PROPOSITION 4.5 If $\mathbf{f}$ is Lipschitz on bounded U, with $U_\delta \subset U$ such that (2.25) holds then there exists $H(\delta) > 0$ such that no point of U_δ is contained in a 2-cycle of the zero-stable method (4.1) with $\rho(-1) \neq 0$ and step-size $h < H(\delta)$.

Proof. Let

$$M = \sup_{\mathbf{y} \in U} \|\mathbf{f}(\mathbf{y})\| \tag{4.9}$$

Suppose $\mathbf{u} \in U_\delta$ is contained in a 2-cycle, then by Theorem 4.4 $\sigma(-1) \neq 0$. Hence if

$$h < \frac{1}{2M} \left| \frac{\rho(-1)}{\sigma(-1)} \right|$$

then (4.6) implies $\mathbf{v} \in U$. The parallelogram law states that

$$\|\mathbf{f}(\mathbf{v}) - \mathbf{f}(\mathbf{u})\|^2 + \|\mathbf{f}(\mathbf{v}) + \mathbf{f}(\mathbf{u})\|^2 = 2(\|\mathbf{f}(\mathbf{v})\|^2 + \|\mathbf{f}(\mathbf{u})\|^2). \tag{4.10}$$

Lipschitz continuity and (4.6) imply that

$$\|\mathbf{f}(\mathbf{v})-\mathbf{f}(\mathbf{u})\| \leq 2hL\left|\frac{\sigma(-1)}{\rho(-1)}\right| \|\mathbf{f}(\mathbf{v})\|.$$

This together with (4.5) implies that (4.10) becomes

$$\|\mathbf{f}(\mathbf{v})\|^2+\|\mathbf{f}(\mathbf{u})\|^2 \leq 2\left(hL\frac{\sigma(-1)}{\rho(-1)}\right)^2 \|\mathbf{f}(\mathbf{v})\|^2,$$

which, together with $\mathbf{f}(\mathbf{v}) \neq 0$, leads to a contradiction when

$$h<\frac{1}{\sqrt{2}L}\left|\frac{\rho(-1)}{\sigma(-1)}\right|. \quad \square$$

PROPOSITION 4.6 Suppose $\mathbf{f}$ is continuous on compact U. With $U_\delta \subset U$ such that (2.25) holds, then given $\varepsilon, \beta>0$ there exists $H(\varepsilon, \beta)>0$ such that if $\mathbf{u} \in U_\delta$ and $\mathbf{u}$ is contained in a 2-cycle of the zero-stable method (4.1) with $\rho(-1) \neq 0$ with $h<H(\varepsilon, \beta)$ then

(i) $\|\mathbf{f}(\mathbf{u})\|, \|\mathbf{f}(\mathbf{v})\|<\varepsilon$

(ii) $\|\mathbf{u}-\mathbf{v}\|<\beta$

where $\mathbf{v}$ is the other point of the two-cycle.

Proof. Since U is compact $\mathbf{f}$ is uniformly continuous on U. Thus given $\varepsilon>0$ there exists $\delta_1>0$ such that $\forall \mathbf{x}, \mathbf{y} \in U$ with $\|\mathbf{x}-\mathbf{y}\|<\delta_1$ it follows that $\|\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{y})\|<\varepsilon$. Let $\delta_2=\min(\delta, \delta_1, \beta)$.

Suppose that $\mathbf{u} \in U_\delta$ is contained in a 2-cycle, then by Theorem 4.4 $\sigma(-1) \neq 0$. Now with M defined by (4.9) suppose

$$h<\frac{2\delta_2}{M}\left|\frac{\rho(-1)}{\sigma(-1)}\right|$$

then (4.6) implies $\|\mathbf{u}-\mathbf{v}\|<\delta_1$ and hence $\|\mathbf{f}(\mathbf{u})-\mathbf{f}(\mathbf{v})\|<\varepsilon$. The result now follows from (4.5) and the triangle inequality. $\square$

The following result follows easily from Proposition 4.5.

THEOREM 4.7 If $\mathbf{f}$ is globally Lipschitz with Lipschitz constant L, the method (4.1) is zero-stable with $\rho(-1) \neq 0$ and

$$h<\frac{1}{\sqrt{2}L}\left|\frac{\rho(-1)}{\sigma(-1)}\right| \tag{4.11}$$

then the method admits no period 2 solutions. $\square$

Remark 4.8 This result ties in well with the existing theory, since if $\rho(-1)=0$ by Example 4.2 trivial bounded spurious solutions exist for all h and the allowed step-size in Theorem 4.7 tends to zero as $\rho(-1) \rightarrow 0$, on the other hand, if $\sigma(-1)=0$ spurious solutions cannot exist and as $\sigma(-1) \rightarrow 0$ the allowed step-size in Theorem 4.7 becomes unbounded.

Now Theorems 3.5, 3.7, 3.8 and Corollarys 3.9 and 3.10 all hold for linear multistep methods (4.1) which are zero-stable with $\rho(-1) \neq 0$. The proofs follow from Proppsitions 4.5 and 4.6 in the same way as the Runge–Kutta results followed from Propositions 3.3 and 3.4. Example 3.6 is also relevant, and shows that bounded period 2 solutions can exist for h arbitrarily small when $\mathbf{f}$ is continuous on $\mathscr{R}^m$.

Note that for implicit methods we have made no assumption on the scheme used to solve (4.1). This points out a fundamental difference between implicit linear multistep methods, for which the above results are a consequence of the method (4.1), and implicit Runge–Kutta methods, for which the equivalent results are a consequence of the iteration scheme used to implement the method, and which by Example 2.8 are not true for arbitrary solutions of the Runge–Kutta equations (2.1–2).

5. Spurious solutions of predictor-corrector methods

Predictor-corrector methods are a popular means of solving the nonlinear equations that occur in the application of implicit ordinary differential equation solvers. A simple predictor-corrector method in PC^m implementation which has been studied in [7, 8] is the following method consisting of a single step of Forward Euler predictor followed by m steps of trapezoidal rule corrector.

$$\begin{aligned} \mathbf{y}_{n+1}^{0} &= \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_n) \\ \mathbf{y}_{n+1}^{k+1} &= \mathbf{y}_n + \frac{h}{2}(\mathbf{f}(\mathbf{y}_n) + \mathbf{f}(\mathbf{y}_{n+1}^{k})) \qquad k = 0, \ldots, m-1 \\ \mathbf{y}_{n+1} &= \mathbf{y}_{n+1}^{m} \end{aligned} \tag{5.1}$$

It is easy to see that (5.1) retains all steady solutions of (1.1). Iserles [7] considered the existence of spurious fixed points of (5.1) when applied to the logistic equation, considered as a function from $\mathscr{C} \to \mathscr{C}$. Spurious equilibria were seen to exist for all values of m, but Iserles observed that if attention was restricted to the real logistic equation then real spurious equilibria occur for m odd but not for m even.

Iserles *et al.* [8] applied bifurcation analysis to (5.1) to prove that the PC^m method (5.1) is $IR^{[1]}$ for m odd and $IR^{[2]}$ for m even. An example was presented, with $f(y) = -1/y$ showing that for this function the method exhibits a spurious fixed point for $m = 2$ and a 2-cycle for $m = 1$. This shows that the necessary conditions for (5.1) to be $R^{[1]}$ (namely m even) or $R^{[2]}$ (m odd) are not sufficient. We will now prove that the method (5.1) is $IR^{[1]}$ for all m, by showing that this method is equivalent to an explicit Runge–Kutta method.

Lemma 5.1 The predictor corrector method (5.1) is equivalent to the $m+1$ stage explicit Runge–Kutta method defined by

$$\begin{aligned} \mathbf{Y}_1 &= \mathbf{y}_n \\ \mathbf{Y}_2 &= \mathbf{y}_n + h\mathbf{f}(\mathbf{Y}_1) \\ \mathbf{Y}_{j+1} &= \mathbf{y}_n + \frac{h}{2}(\mathbf{f}(\mathbf{Y}_1) + \mathbf{f}(\mathbf{Y}_j)), \qquad j = 2, \ldots, m \\ \mathbf{y}_{n+1} &= \mathbf{y}_n + \frac{h}{2}(\mathbf{f}(\mathbf{Y}_1) + \mathbf{f}(\mathbf{Y}_{m+1})). \end{aligned} \tag{5.2}$$

Proof. Observe that $\mathbf{Y}_{j+2} = \mathbf{y}^j_{n+1}$ for $j = 0, \ldots, m-1$. □

THEOREM 5.2 The predictor corrector method (5.1) is $IR^{[1]}$ for all $m \geq 1$.

Proof. The Runge–Kutta method (5.2) is not equivalent to the Forward Euler method for $m \geq 1$. (Since $b_{m+1} \neq 0$ and $a_{i,i-1} \neq 0$ for all i the method does not produce the same solution sequence as any Runge–Kutta method with less than $m+1$ stages.) Hence by Theorem 2.1 it is $IR^{[1]}$. □

Since the Forward Euler method is $R^{[1]}$ if we take $m = 0$ in (5.1) we do obtain an $R^{[1]}$ method. Thus in some senses the corrector could be said to be badly named, since it destroys the property of being $R^{[1]}$. The dependence on the parity of m for the method to be $R^{[1]}$ or $R^{[2]}$ observed in [7] resulted from consideration of the logistic equation, but as was observed in [5] this approach is not sufficient to determine regularity. The above result confirms this.

The bifurcation analysis used in [8] could be used to study the regularity or otherwise of general Adams–Bashforth/Adams–Moulton predictor-corrector methods in PC^m mode. At first sight it would appear that the 'trick' of Lemma 5.1 could not be applied to more general methods. In fact we can use this technique to show that other PC^m methods allow the existence of spurious equilibria.

Consider the two-step Adams–Bashforth/Adams–Moulton predictor-corrector method (5.3) in PC^m implementation.

$$\begin{aligned}
\mathbf{y}^0_{n+1} &= \mathbf{y}_n + \frac{h}{2}(3\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{y}_{n-1})) \\
\mathbf{y}^{k+1}_{n+1} &= \mathbf{y}_n + \frac{h}{12}(5\mathbf{f}(\mathbf{y}^k_{n+1}) + 8\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{y}_{n-1})), \qquad k = 0, \ldots, m-1 \\
\mathbf{y}_{n+1} &= \mathbf{y}^m_{n+1}
\end{aligned} \tag{5.3}$$

Suppose that $\hat{\mathbf{y}}$ is a steady solution of (5.3). Then identifying $\mathbf{y}_n$ and $\mathbf{y}_{n-1}$ in (5.3) it follows that $\hat{\mathbf{y}}$ is also a steady solution of (5.4).

$$\begin{aligned}
\mathbf{y}^0_{n+1} &= \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_n) \\
\mathbf{y}^{k+1}_{n+1} &= \mathbf{y}_n + \frac{h}{12}(5\mathbf{f}(\mathbf{y}^k_{n+1}) + 7\mathbf{f}(\mathbf{y}_n)), \qquad k = 0, \ldots, m-1 \\
\mathbf{y}_{n+1} &= \mathbf{y}^m_{n+1}
\end{aligned} \tag{5.4}$$

But (5.4) is equivalent to the explicit Runge–Kutta method (5.5), (proof as Lemma 5.1).

$$\begin{aligned}
\mathbf{Y}_1 &= \mathbf{y}_n \\
\mathbf{Y}_2 &= \mathbf{y}_n + h\mathbf{f}(\mathbf{Y}_1) \\
\mathbf{Y}_{j+1} &= \mathbf{y}_n + \frac{h}{12}(7\mathbf{f}(\mathbf{Y}_1) + 5\mathbf{f}(\mathbf{Y}_j)), \qquad j = 2, \ldots, m \\
\mathbf{y}_{n+1} &= \mathbf{y}_n + \frac{h}{12}(7\mathbf{f}(\mathbf{Y}_1) + 5\mathbf{f}(\mathbf{Y}_{m+1}))
\end{aligned} \tag{5.5}$$

The explicit Runge–Kutta method (5.5) is not equivalent to the Forward Euler method and thus by Theorem 2.1 is $IR^{[1]}$. Hence for some $\mathbf{f}$ (5.5) admits a solution with $\mathbf{y}_{n+1} = \mathbf{y}_n = \hat{\mathbf{y}}$ but $\mathbf{f}(\hat{\mathbf{y}}) \neq 0$. $\mathbf{y}_{n+1} = \mathbf{y}_n = \hat{\mathbf{y}}$ will also be a solution of (5.4), since (5.5) and (5.4) are equivalent, and hence $\hat{\mathbf{y}}$ is a spurious steady solution of (5.3). Therefore the PC^m method (5.3) is $IR^{[1]}$.

The same technique (identifying $\mathbf{y}_n, \ldots, \mathbf{y}_{n-k+1}$ and showing equivalence to an explicit Runge–Kutta method) can be applied to any predictor-corrector method which is based on linear multistep methods, and in PC^m implementation, to show the existence of spurious steady solutions, unless the method is equivalent to the Forward Euler method. Thus we have the order barrier. *The highest possible order of a $R^{[1]}$ PC^m method based on linear multistep methods is* 1. In fact it is easy to see that the Runge–Kutta method 'corresponding' to any PC^m method will have $b_{m+1} \neq 0$ and $a_{i,i-1} \neq 0$ for all i and that hence it cannot be equivalent to any explicit Runge–Kutta method with fewer stages. In particular it is not equivalent to the Forward Euler method and by appealing to Theorem 2.1 again we have

THEOREM 5.3 Every predictor-corrector method in PC^m mode, which consists of one step of an explicit linear multistep predictor and m steps of an implicit linear multistep corrector (and in particular every Adams–Bashforth/Adams–Moulton PC^m method) is $IR^{[1]}$. □

Although we have shown that all these methods admit spurious fixed solutions, because of the equivalence between these solutions and the spurious fixed solutions of the 'equivalent' explicit Runge–Kutta methods the results of Section 3 all apply to spurious fixed solutions of predictor-corrector methods. In particular if $\mathbf{f}$ is globally Lipschitz spurious solutions cannot exist for h arbitrarily small, and if $\mathbf{f}$ is locally Lipschitz and spurious solutions exist for h arbitrarily small then they become unbounded in norm as $h \to 0$.

We have not shown whether general PC^m methods are $R^{[2]}$ or $IR^{[2]}$, nor are we able to apply the results of Section 4 to the spurious period 2 solutions (if they exist) of these methods except for the specific method (5.1), which by Lemma 5.1, is an explicit Runge–Kutta method.

Suppose now that we apply a predictor-corrector method in PC^∞ mode, that is we iterate the corrector to convergence. For example consider the scheme

$$\begin{aligned} \mathbf{y}_{n+1}^0 &= \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_n) \\ \mathbf{y}_{n+1}^{k+1} &= \mathbf{y}_n + \frac{h}{2}(\mathbf{f}(\mathbf{y}_n) + \mathbf{f}(\mathbf{y}_{n+1}^k)) \qquad k = 0, 1, \ldots \\ \mathbf{y}_{n+1} &= \lim_{k\to\infty} \mathbf{y}_{n+1}^k \end{aligned} \tag{5.6}$$

Allowing $k \to \infty$ in (5.6) we obtain $\mathbf{y}_{n+1} = \mathbf{y}_n + (h/2)(\mathbf{f}(\mathbf{y}_n) + \mathbf{f}(\mathbf{y}_{n+1}))$. Thus in this case the iteration solves the implicit trapezoidal rule and the PC^∞ method inherits the regularity characteristics of that method. The trapezoidal rule is known to be $R^{[1,2]}$ (see [12]), thus so is the scheme (5.6). If we now consider more general Adams–Bashforth/Adams–Moulton methods in PC^∞ mode, we see that all these methods are equivalent to the linear multistep method which defines the corrector. Thus these methods are all $R^{[1]}$ and Theorem 4.4 identifies the methods which are $R^{[2]}$. For $IR^{[2]}$ methods the results of the previous section apply.

In practice to solve (5.6) in finite time the iteration must be terminated after some number of steps, and thus our study of (5.1) might lead us to expect spurious steady solutions after all. Careful application should however prevent this, since although we know that for any k we may have $\mathbf{y}_{n+1}^k = \mathbf{y}_n$ with $\mathbf{f}(\mathbf{y}_n) \neq 0$ since the implicit trapezoidal rule is $R^{[1]}$ in this case we will have $\mathbf{y}_{n+1}^{k+1} \neq \mathbf{y}_{n+1}^k$ and so convergence will not have occurred. However rigorous analysis of the existence of spurious solutions when the equations defining the method are solved approximately are beyond the scope of this paper.

The above discussion suggests that iterating the corrector to convergence, and thus retaining the regularity characteristics of the corrector, may be a good means of solving implicit methods, with good reproduction of the long term dynamics provided that the corrector is regular. However if PC^m methods are used to solve for long time behaviour of a system (1.1) we may expect spurious dynamics to occur.

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