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A Hopf Bifurcation Theorem for Difference Equations Approximating a Differential Equation

By

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Abstract. If an ordinary differential equation is discretizised near an asymptotically stable stationary solution with a pair of imaginary eigenvalues by Euler's method with constant step length h, small invariant attracting cycles of radius $O(h^{1/2})$ will appear. This Hopf bifurcation theorem is applied to prove the existence of limit cycles in certain difference equations occurring in biomathematics (hypercycle, two loci-two alleles) and is also extended to general Runge—Kutta methods.

1. Introduction

Given an autonomous differential equation

$$\frac{dx}{dt} = f(x), \tag{1.1}$$

defined in some open set in $\mathbb{R}^n$, the "simplest integration procedure" consists in replacing the differential quotient $\frac{dx}{dt}$ by a difference quotient $\frac{\Delta x}{\Delta t} = \frac{x(t+\varepsilon) - x(t)}{\varepsilon}$. Thus we are led to consider the maps

$$T_\varepsilon : x \to x + \varepsilon f(x) \quad \text{for small} \quad \varepsilon > 0\,. \tag{1.2}$$

Now the question arises, how well the asymptotic behaviour of (1.1) carries over to (1.2) for small ε. Since it would be a difficult task to compare the global dynamics we restrict ourselves to local questions.

Obviously the differential equation (1.1) and the maps T_ε have the same fixed points. Suppose $x = 0$ to be a fixed point and $f(x)$ to have the form

$$f(x) = A\,x + O(\|x\|^2)\,.$$

Then

$$T_\varepsilon x = (1 + \varepsilon A)\,x + \varepsilon\, O(\|x\|^2)\,.$$

So λ is an eigenvalue of A, iff $1 + \varepsilon\lambda$ is an eigenvalue of the linearization of T_ε. Therefore, if A is hyperbolic (i. e. no eigenvalue has zero real part), the local behaviour near $x = 0$ will be the same for the flow (1.1) and the maps T_ε provided ε is small enough.

But if A is not hyperbolic this need no longer be true. Suppose A has a pair of purely imaginary eigenvalues. Then 0 will be unstable for (1.2) for every $\varepsilon > 0$, although it could be asymptotically stable for (1.1). It is the object of this paper to determine the asymptotic behaviour of the maps T_ε in this case. We will show in § 2, that due to a kind of Hopf bifurcation invariant attracting circles of radius $O(\varepsilon^{1/2})$ appear.

In § 3 we will apply this result to some equations used in biomathematics.

In § 4 we generalize our theorem to other discretization methods, in particular general explicit m-stage Runge—Kutta procedures.

2. The Hopf Bifurcation Theorem

Theorem 1: *Consider an ordinary differential equation $\dot{x} = f(x)$, defined in some neighbourhood U of 0 in $\mathbb{R}^n$, which satisfies*

(i) *$f(0) = 0$, $Df(0)$ has two simple imaginary eigenvalues $\pm i\omega$, the rest of the spectrum has negative real part.*

(ii) *0 is a "weakly stable" fixed point (see the following remark). Then for any family of maps T_ε satisfying*

$$T_\varepsilon x = x + \varepsilon f(x) + O(\varepsilon^2 \|x\|^2) \quad \text{for} \quad \varepsilon > 0,\ \|x\| \to 0\,, \qquad (2.1)$$

there exists a family of closed curves $\gamma_\varepsilon (0 < \varepsilon < \varepsilon_0)$ surrounding the origin, invariant and attracting for T_ε, which are of radius $O(\varepsilon^{1/2})$ in general.

Remark: "weak stability" means roughly speaking asymptotic stability which can be recognized already from the terms of degree $\leqslant h$ for some natural number h. We do not want to go into the details and refer the interested reader to the paper of NEGRINI and SALVADORI [16] who make a detailed study of this concept of h-asymptotic stability. E. g. the "vague attractor" condition of [13, 14] corresponds to $h = 3$. For analytic $f(x)$, "weak stability" is the same as asymptotic stability (at least in the two-dimensional case), but not for $C^\infty f(x)$.

Proof: We use the standard method for proving the Hopf bifurcation theorem for maps, as proposed by RUELLE and TAKENS

[17], and worked out in detail by LANFORD [13] and IOOSS [11]. Since we cannot apply the center manifold theorem directly (although it would be possible after some refinements) we will apply the procedure to the whole n-dimensional equation.

Before writing (1.1) in normal form we have to look how a change of coordinates transforms the maps T_ε:

Suppose $\Phi: x \to y = \Phi(x)$ is a local diffeomorphism. Then (1.1) reads in y-coordinates

$$\dot{y} = D\Phi(x)\dot{x} = D\Phi(x) f(x)$$

and the maps T_ε are transformed to

$$\begin{aligned}\tilde{T}_\varepsilon y &= \Phi \circ T_\varepsilon \circ \Phi^{-1}(y) = \Phi(T_\varepsilon x) = \Phi(x + \varepsilon f(x)) = \\ &= \Phi(x) + \varepsilon D\Phi(x)(f(x) + \frac{\varepsilon^2}{2} D^2\Phi(\tilde{x})(f(x), f(x)) = \\ &= y + \varepsilon \dot{y} + O(\varepsilon^2 \| y \|^2)\end{aligned}$$

So, after making a change of coordinates, we have to consider maps T_ε, which differ from (1.2) by order $O(\varepsilon^2 \| x \|^2)$. To illustrate this, the time-ε-map of (1.1), for which the theorem will of course not apply, satisfies only $x(\varepsilon) = x + \varepsilon \dot{x} + O(\varepsilon^2 \| x \|)$.

Now a linear change of variables takes (1.1) into

$$\begin{cases} \dot{z} = i\omega z + \text{higher order terms} \\ \dot{v} = A v + h.o.t. \end{cases} \tag{2.2}$$

where the complex variable z comes from the two-dimensional eigenspace of the critical eigenvalues $\pm i\omega$ and v from the eigenspace of the rest of the spectrum. Since this has strictly negative real part, there are no further resonances for the critical eigenvalues $\pm i\omega$ than the usual ones. So according to the general theory of normal forms (see [3]), by a nonlinear change of variables, we arrive at

$$\begin{aligned} \dot{z} &= i\omega z + \sum_{j=1}^{2k} \alpha_j z |z|^{2j} + O(|z| + |v|)^{4k+2} \\ \dot{v} &= A v + O(|z|^2 + |v|^2). \end{aligned} \tag{2.3}$$

We suppose $\alpha_j = a_j + i b_j$ with $a_1 = a_2 = \ldots = a_{k-1} = 0$, and according to our weak stability assumption: $a_k < 0$. Then the maps $T_\varepsilon(z, v) = (z_\varepsilon, v_\varepsilon)$ take the form

$$z_\varepsilon = (1 + i\varepsilon\omega) z + \varepsilon \sum_{j=1}^{2k} \alpha_j z|z|^{2j} + O(\varepsilon(|z| + |v|)^{4k+2} + \varepsilon^2(|z|^2 + |v|^2))$$

$$v_\varepsilon = (1 + \varepsilon A) v + \varepsilon O(|z|^2 + |v|^2).$$

Now the terms linear in ε are already in best possible form, but it is necessary to improve also the ε^2-terms. It is easy to check that by an ε-dependent change of the form $z' = z + \varepsilon\varphi(z, v)$ one can eliminate every ε^2-term (besides the resonants $z|z|^{2j}$) one wants, without destroying the ε-terms. So we arrive with $\alpha_j(\varepsilon) = \alpha_j + \varepsilon\alpha_j'$ at

$$z_\varepsilon = (1 + i\varepsilon\omega) z + \varepsilon \sum_{j=1}^{2k} \alpha_j(\varepsilon) z|z|^{2j} + O(\varepsilon(|z|^2 + |v|^2)^{2k+1} + \\ + \varepsilon^2(|z|^2 + |v|^2)^{k+1} + \varepsilon^3(|z|^2 + |v|^2))$$

$$v_\varepsilon = (1 + \varepsilon A) v + \varepsilon O(|z|^2 + |v|^2).$$

Substitution to polar coordinates $z = re^{i\theta}$ gives

$$r_\varepsilon^2 = r^2[(1 + \varepsilon \sum_{j=1}^{2k} a_j(\varepsilon) r^{2j})^2 + \varepsilon^2(\omega + \sum_{j=1}^{2k} b_j r^{2j})^2 + \frac{1}{r} O(\ldots)]$$

$$\theta_\varepsilon = \theta + \varepsilon(\omega + \sum_{j=1}^{2k} b_j(\varepsilon) r^{2j})(1 - \varepsilon \sum_{j=1}^{2k} a_j(\varepsilon) r^{2j}) + \frac{1}{r} O(\ldots)$$

$$v_\varepsilon = (1 + \varepsilon A) v + \varepsilon O(r^2 + |v|^2).$$

Writing $v = rw$ leads to

$$r_\varepsilon = r\Big[1 + \varepsilon \sum_{j=1}^{2k} a_j(\varepsilon) r^{2j} + \frac{\varepsilon^2}{2}(\omega + \sum_{j=1}^{2k} b_j r^{2j})^2 + \\ + O(\varepsilon r^{4k+1} + \varepsilon^2 r^{2k+1} + \varepsilon^3 r + \varepsilon^4)\Big]$$

$$\theta_\varepsilon = \theta + \varepsilon(\omega + \sum_{j=1}^{2k} b_j(\varepsilon) r^{2j}) + O(\varepsilon r^{4k+1} + \varepsilon^2 r^{2k} + \varepsilon^3)$$

$$w_\varepsilon = (1 + \varepsilon A) w + O(\varepsilon r + \varepsilon^2).$$

Truncating this map by neglecting the O-terms we obtain an invariant attracting circle $r = r_0(\varepsilon)$, $w = 0$ as the solution of

$$\sum_{j=1}^{2k} a_j(\varepsilon) r_0^{2j}(\varepsilon) = -\frac{\varepsilon}{2}(\omega + \sum_{j=1}^{2k} b_j r_0^{2j}(\varepsilon))^2. \tag{2.4}$$

Hence

$$r_0(\varepsilon) = \left(-\frac{\varepsilon\,\omega^2}{2\,a_k}\right)^{1/(2k)} + O(\varepsilon^{3/(2k)}) \,. \tag{2.5}$$

Therefore the perturbations are of $o(\varepsilon^3)$ and the expansion of $r_0(\varepsilon)$ in terms of powers of $\varepsilon^{1/2k}$ will persist for the first $2k$ terms. So our last scaling is $r = r_0(\varepsilon)(1 + \varepsilon x)$ which gives

$$\begin{aligned} x_\varepsilon &= x(1 - k\,\varepsilon^2\,\omega^2) + \varepsilon^{2+1/(2k)} f(x, \theta, w, \varepsilon) \\ \theta_\varepsilon &= \theta + \Omega(\varepsilon) + \varepsilon^{2+1/(2k)} g(x, \theta, w, \varepsilon) \\ w_\varepsilon &= (1 + \varepsilon A)\, w + \varepsilon^{1+1/(2k)} h(x, \theta, w, \varepsilon) \end{aligned} \tag{2.6}$$

with $\Omega(\varepsilon) = \varepsilon(\omega + \sum_{j=1}^{2k} b_j r_0(\varepsilon)^{2j})$, and w lies in some $(n-2)$-dimensional subspace $V \subseteq \mathbb{R}^n$.

Now the rest of the proof runs essentially as in [11, p. 34ff.]:

Let us define a function space, where $T^1 = \mathbb{R}\,|\,2\pi\mathbb{Z}$

$$\mathscr{E} = \{(x, w) : T^1 \to \mathbb{R} \times V;\ |x(\theta)| \leqslant 1,\ \|w(\theta)\| \leqslant 1,$$
$$\max(|x(\theta_1) - x(\theta_2)|,\ \|w(\theta_1) - w(\theta_2)\|) \leqslant |\theta_1 - \theta_2|\} \,.$$

With the usual distance

$$d((x_1, w_1), (x_2, w_2)) = \|(x_1 - x_2, w_1 - w_2)\|$$
$$\|(x, w)\| = \max_{\theta \in T^1}(|x(\theta)|, \|w(\theta)\|) \,,$$

$\mathscr{E}$ becomes a complete metric space.

The idea is now to show that for $(x, w) \in \mathscr{E}$ we can write

$$T_\varepsilon(x(\theta), \theta, w(\theta)) = (\hat{x}(\theta_\varepsilon), \theta_\varepsilon, \hat{w}(\theta_\varepsilon))$$

for some $(\hat{x}, \hat{w}) \in \mathscr{E}$. Then it will be sufficient to prove the existence of a fixed point in $\mathscr{E}$ of the map $\mathfrak{F} : (x, w) \to (\hat{x}, \hat{w})$. For this it is useful to know that f, g, h are C^1 in $[0, 1] \times T^1 \times B_V$, where B_V is the unit ball of V, this being valid uniformly for ε small enough.

The proof works in the following way:

1st step: Consider $(x, w) \in \mathscr{E}$. Then the map $\theta \to \theta_\varepsilon = \Theta_{x,w}(\theta)$ is a bilipschitz homeomorphism of T^1, such that $\Theta_{x,w}^{-1}$ has a Lipschitz constant $\leqslant 1 + O(\varepsilon^{2+1/(2k)})$.

2nd step: Now we can define $(\hat{x}, \hat{w})$ by

$$\hat{x}(\Theta) = (1 - \varepsilon^2 k \omega^2) x(\theta) + \varepsilon^{2+1/(2k)} f(x(\theta), \theta, w(\theta), \varepsilon)$$

$$\hat{w}(\Theta) = (1 + \varepsilon A) w(\theta) + \varepsilon^{1+1/(2k)} h(x(\theta), \theta, w(\theta), \varepsilon)$$

where $\theta = \Theta^{-1}_{x,w}(\Theta)$.

It is now easy to prove that $(\hat{x}, \hat{w}) \in \mathscr{E}$, so we defined a map on $\mathscr{E}$. Then it is possible to prove that this map is a strict contraction for ε small enough, thanks to the facts that $1 - \varepsilon^2 \omega^2 k$ is perturbed only by terms of order $\varepsilon^{2+1/(2k)}$, and that $1 + \varepsilon A$ is a contraction of rate $1 - \sigma\varepsilon$ perturbed by terms of order $\varepsilon^{1+1/(2k)}$. These perturbations come from f, h and from the dependence of $\Theta^{-1}_{x,w}(\Theta)$ in (x, w), which can be estimated as

$$|\Theta^{-1}_{x_1,w_1}(\Theta) - \Theta^{-1}_{x_2,w_2}(\Theta)| \leqslant O(\varepsilon^{2+1/(2k)}) \| (x_1, w_1) - (x_2, w_2) \|$$

for $(x_i, w_i) \in \mathscr{E}$, $i = 1, 2$.

The details of the proof are straightforward.

3. Applications to Biomathematics

When modelling the time evolution of the state of biological populations, e. g. population numbers or frequencies of certain types within one population, one has two principal possibilities: to assume either separated generations and work with a discrete time model described by difference equations, or overlapping generations leading to a continuous time model described by differential equations. Generally both possibilities are treated parallely in biomathematics. (Often biologists prefer discrete time since it is easier to simulate on a computer whereas mathematicians prefer continuous time because differential equations are easier to analyze.) In many cases, although arising from different models, these differential equations can be obtained formally from the difference equations by just replacing $x' - x$, the increase from one generation to the next, by $\dot{x} = dx/dt$, or the simple limit process discussed above. We will give two simple examples in the following:

Let us start with equations of the form

$$x_i' = x_i \cdot \sum_{j=1}^{n} \alpha_{ij} x_j / \Psi, \quad i = 1, \ldots, n, \quad \Psi = \sum_{i,j=1}^{n} \alpha_{ij} x_i x_j \tag{3.1}$$

and

$$\dot{x}_i = x_i(\sum_{j=1}^{n} a_{ij}x_j - \Phi), \quad i = 1, \ldots, n, \quad \Phi = \sum_{i,j=1}^{n} a_{ij}x_i x_j \qquad (3.2)$$

defined on the probability simplex

$$S_n = \{x \in \mathbb{R}^n : \sum_{i=1}^{n} x_i = 1, x_i \geqslant 0\}.$$

These equations were first introduced by Fisher in the 1930's in the special case of symmetric matrices $\alpha_{ij} = \alpha_{ji}$. They simulate the genetic state of a Mendelian population under the force of selection, based on the Hardy—Weinberg law. The x_i are the frequencies of alleles $A_i (i = 1, \ldots, n)$ at one gene locus and α_{ij} resp. a_{ij} is the fitness of the genotype $A_i A_j$. More exactly: α_{ij} = probability of surviving of an $A_i A_j$-individual into the next season and a_{ij} = difference between its birth and death rate.

Neglecting the different biological meanings of α_{ij} and a_{ij}, we will see now that formally (3.1) approximates (3.2): For this end, choose $\alpha_{ij} = a_{ij} + C$ with C a large constant. Then (3.1) reads

$$x_i' - x_i = \frac{x_i(\sum_j \alpha_{ij}x_j - \Psi)}{\Psi} = x_i \frac{\sum_j a_{ij}x_j - \Phi}{C + \Phi}.$$

Now let $p \in S_n$ be a fixed point of (3.2) and choose $\varepsilon = (C + \Phi(p))^{-1}$, then

$$\frac{1}{C + \Phi(x)} = \varepsilon\left(1 + \frac{\Phi(p) - \Phi(x)}{C + \Phi(x)}\right) = \varepsilon\left(1 + \frac{O(\|x - p\|)}{C + \Phi(p)}\right) =$$

$$= \varepsilon + O(\varepsilon^2 \|x - p\|).$$

Hence $x_i' - x_i = \varepsilon \dot{x}_i + O(\varepsilon^2 \|x - p\|^2)$ and (3.1) and (3.2) are in the right relation to apply our theorem at the neighbourhood of p.

However the *Fundamental Theorem of Natural Selection* [1, 5] says that for both (3.1) and (3.2), with symmetric (α_{ij}) and (a_{ij}), the mean fitness Ψ resp. Φ of the population is constantly increasing. So our Hopf bifurcation theorem is not applicable to this situation. But it works for two slight extensions of these equations.

The first is simply to admit nonsymmetric matrices (α_{ij}) and (a_{ij}). Equations (3.1) and (3.2) play then an important role at two different periods of the evolutionary scale. They describe the dynamics of catalytic networks of selfreplicating macromolecules as studied by EIGEN and SCHUSTER [4] in their theory of selforganization of matter

(see also [10, 19]). Here the x_i represent the proportions of the selfreplicating units in an evolution reactor and a_{ij} measures the catalytic action of the j-th species to the replication of the i-th species.

Maynard Smith proposed (3.1) and (3.2) as dynamics for an evolutionary game after having successfully applied game theory to explain the evolution of animal behaviour. x_i then denote the frequencies of players of different behavioural strategies (like "hawk", "dove", retaliator, etc.) and α_{ij} resp. a_{ij} is the payoff for an i-player after a contest against an j-player. [15, 18, 21, 23].

Further the differential equation (3.2) has been shown [8] to be equivalent to the ubiquitous Lotka—Volterra equations. Of course (3.2) is easier to analyze than (3.1). In particular one can show [10, 23] that (3.2) admits (supercritical) Hopf bifurcations if $n \geqslant 4$. The simplest example is the Eigen—Schuster "hypercycle"-equation

$$\dot{x}_i = x_i(x_{i-1} - \Phi) \quad i = 1, \ldots, n. \tag{3.3}$$

For $n = 4$ the stationary solution ($x_i = \frac{1}{4}$) is asymptotically stable, as is easily seen using $P = x_1 x_2 x_3 x_4$ as a Lyapunov function, but has a pair of purely imaginary eigenvalues. So it is a good candidate for our theorem. Since the above approximation argument works for non-symmetric matrices too, we may conclude that the corresponding difference equation

$$x_i' = x_i \frac{C + x_{i-1}}{C + \Phi}, \quad C > 0 \tag{3.4}$$

which was studied in [9], has an invariant attracting curve for each large C (if $n = 4$), of radius $\approx C^{-1/2}$. (In fact our general theorem was motivated by numerical simulations of this particular equation.)

Returning to population genetics again, a second generalization of our first example would be to consider alleles at different loci. Then the possibility of cross overs produces an additional term in (3.1) and (3.2): the recombination field [1]. The simplest example is two alleles at two different loci, say A_1, A_2 at the first and B_1, B_2 at the second, representing (somewhat oversimplified) e. g. blue and brown color of the eyes, and blond and black color of hair. So let x_1, x_2, x_3, x_4 be the frequencies of the four gametes $A_1 B_1$, $A_1 B_2$, $A_2 B_1$ and $A_2 B_2$; α_{ij} resp. a_{ij} the average fitness of an individual carrying the i-th and j-th gamete; r the recombination fraction (= probability for a cross over), $D = x_1 x_4 - x_2 x_3$ the measure of linkage disequilibrium and $\xi_1 = = -\xi_2 = -\xi_3 = \xi_4 = -1$. Then the time evolution is governed by

$$\dot{x}_i = x_i(\sum_{j=1}^{4} a_{ij}x_j - \Phi) + r\xi_i D \qquad i = 1,\ldots,4 \tag{3.5}$$

for overlapping generations and by

$$\Psi x_i' = x_i(\sum_{j=1}^{4} \alpha_{ij}x_j) + r\xi_i D \tag{3.6}$$

for separated generations.

For these equations the "Fundamental Theorem of Natural Selection" is in general no longer true, and in fact they are very difficult to analyze. Only recently the occurrence of (supercritical) Hopf bifurcations has been shown by AKIN [2] for (3.5), and HASTINGS [7] has found them in (3.6) by numerical simulations. Since the same argument as above shows that (3.6) are suitable approximations of (3.5), our theorem and Akin's result together give an exact proof for the existence of "limit cycles" also in the discrete time model (3.6).

4. Generalization to Other Discretization Methods

In this section we will investigate to what extent our Hopf bifurcation theorem carries over to more refined discretization methods than the simple Euler procedure. We consider general (explicit) m-stage Runge—Kutta schemes

$$T_h x = x + h\sum_{i=1}^{m} c_i f(x_i) \tag{4.1}$$

with $\sum_{i=1}^{m} c_i = 1$ for the differential equation $\dot{x} = f(x)$, where the auxiliary values x_i are given recursively by

$$\begin{aligned} x_1 &= x \\ x_2 &= x + h a_{21} f(x_1) \\ &\vdots \\ x_m &= x + h\sum_{j=1}^{m-1} a_{mj} f(x_j) \end{aligned} \tag{4.2}$$

Again the first thing we do is to estimate the error which is produced by a change of coordinates $\Phi: x \to y = \Phi(x)$ for the discretization maps T_h:

$$\tilde{T}_h y = \Phi \circ T_h \circ \Phi^{-1}(y) = \Phi(T_h x) =$$

$$= \Phi(x) + D\Phi(x) h \sum c_i f(x_i) + \frac{h^2}{2} D^2 \Phi(\tilde{x})(\ldots, \ldots) =$$

$$= y + h \sum c_i D\Phi(x) f(x_i) + O(h^2 x^2).$$

The discretization for the transformed differential equation $\dot{y} = D\Phi(x) f(x) = \tilde{f}(y)$ is given by

$$T_h y = y + h \sum c_i \tilde{f}(y_i) = y + h \sum c_i D\Phi(\xi_i) f(\xi_i)$$

with $\xi_i = \Phi^{-1}(y_i)$. We now show by induction

$$D\Phi(\xi_i) f(\xi_i) = D\Phi(x) f(x_i) + O(h x^2).$$

We have

$$\xi_i = \Phi^{-1}(y_i) = \Phi^{-1}(y + h \sum_j a_{ij} \tilde{f}(y_j)) =$$

$$= \Phi^{-1}(y) + h D\Phi^{-1}(y) \cdot \sum_j a_{ij} \tilde{f}(y_j) + O(h^2 y^2) =$$

$$= x + h D\Phi(x)^{-1} \sum_j a_{ij} D\Phi(\xi_j) f(\xi_j) + O(h^2 y^2)$$

which gives by the induction hypothesis

$$= x + h \sum_j a_{ij} f(x_j) + O(h^2 x^2) =$$

$$= x_i + O(h^2 x^2).$$

Hence

$$\tilde{f}(y_i) = D\Phi(\xi_i) f(\xi_i) = D\Phi(\xi_i) f(x_i) + O(h^2 x^2) =$$
$$= D\Phi(x) f(x_i) + O(h x) f(x_i) + O(h^2 x^2) =$$
$$= D\Phi(x) f(x_i) + O(h x^2).$$

This shows that as for Euler's method, the maps T_h differ at most with error $O(h^2 x^2)$ after a change of coordinates near a fixed point of the differential equation $\dot{x} = f(x)$. The same is true also for general implicit RK-schemes.

Now we apply this RK-procedure to the normal form as in § 2

$$\begin{cases} \dot{z} = \lambda z + \alpha z |z|^2 + O(|z| + |v|)^5 \\ \dot{v} = A v + O(|z|^2 + |v|^2) \end{cases} \tag{4.3}$$

where we suppose $\lambda = i\omega$ and $\alpha = a + ib$ with $a < 0$. (To simplify the

calculations we restrict ourselves here to the "vague attractor" case $k = 1$ of § 2.)

It is easy to see that the vector field at the auxiliary values is given by

$$f(z_i, v_i) = (\lambda_i z + \alpha z|z|^2 + O(h|z|^3 + (|z| + |v|)^5), \\ A_i v + O(|z|^2 + |v|^2))$$

with

$$\lambda_i = \lambda(1 + h\sum_{j=1}^{i-1} a_{ij}\lambda_j)$$

and

$$A_i = (1 + h\sum_{j=1}^{i-1} a_{ij} A_j).$$

So the discretization map $T_h(z, v) = (z_h, v_h)$ takes the form

$$\begin{cases} z_h = g(h\lambda) z + h\alpha z|z|^2 + O(h^2|z|^3 + h(|z| + |v|)^5 + h^2(|z|^2 + |v|^2)) \\ v_h = g(hA) v + h O(|z|^2 + |v|^2) \end{cases}$$

where

$$g(h\lambda) = 1 + h\sum_{i=1}^{\infty} c_i \lambda_i .$$

This function $g(x) = 1 + x + O(x^2)$ is the "growth function" [20, p. 131] of the RK-scheme. It is polynomial for explicit RK-schemes and a rational function for implicit schemes. It actually tells how the scheme acts on *linear* differential equations: For $\dot{x} = \lambda x$, one has $T_h x = g(h\lambda) x$.

As in § 2 it is necessary at this step to improve the $O(h^2)$-terms: Using a change of coordinates $z' = z + h A_2(z, v)$ we can remove the h^2-terms which are of degree 2 also in z, v. This leads to

$$z_h = g(h\lambda) z + h\alpha z|z|^2 + O(h^2(|z| + |v|)^3 + h(|z| + |v|)^5)$$
$$v_h = g(hA) v + h O(|z|^2 + |v|^2)$$

Now introduce polar coordinates $z = r e^{i\theta}$ and set $v = r w$ to obtain

$$r_h^2 = r^2[|g(h\lambda)|^2 + 2ahr^2 + O(hr^4 + h^2 r^2)]$$
$$\theta_h = \theta + \operatorname{Im} g(h\lambda) + bhr^2 + O(hr^4 + h^2 r^2) \qquad (4.4)$$
$$w_h = g(hA) w + h O(r).$$

The rest of the analysis depends essentially on the behaviour of the function $g(x)$ for imaginary values: $|g(ix)|^2$ will be of the form

$$|g(ix)|^2 = 1 + Gx^{2p} + O(x^{2p+2}) \quad \text{with} \quad G \neq 0. \tag{4.5}$$

Then the truncated map (4.4) (without the O-terms) has an attracting invariant circle for small $h > 0$, given by

$$|g(ih\omega)|^2 - 1 + 2ahr^2 = 0 \quad \text{and} \quad w = 0$$

or

$$r_0(h)^2 = \frac{1 - |g(ih\omega)|^2}{2ah} = -\frac{G\omega^{2p}}{2a} h^{2p-1} + O(h^{2p+1}) \tag{4.6}$$

which exists provided $G > 0$ (since $a < 0$).

Scaling finally $r = r_0(h)(1 + h^{1/2}x)$ leads to the desired form (2.6) of the map for which the same fixed argument as indicated in § 2 works again:

$$\begin{aligned} x_h &= x(1 - Gh^{2p}\omega^{2p}) + O(h^{2p+1/2}) \\ \theta_h &= \theta + \Omega(h) + O(h^{2p+1/2}) \\ w_h &= g(hA)w + O(h^{p+1/2}) \end{aligned} \tag{4.7}$$

with $\Omega(h) = \operatorname{Im} g(ih\omega) + bhr_0(h)^2$.

So we have shown the following generalization of our Theorem 1 in § 2:

Theorem 2: *Apply a Runge—Kutta scheme T_h with growth function $g(x)$ satisfying* (4.5) *with $G > 0$ to a differential equation $\dot{x} = f(x)$ which fulfills conditions* (i) *and* (ii) *of Theorem 1. Then there exists a family of closed curves γ_h for small $h > 0$, surrounding the origin, invariant and attracting for T_h, of radius $O(h^{p-1/2})$.*

So we see that essentially the same statement holds as in Theorem 1 (but the circles are smaller in general), provided only that the constant G from (4.5) is positive, that means the growth function takes absolute values greater than 1 on the imaginary axis near 0. This is equivalent to the fact that the "region of absolute stability", i.e. the set $\{x \in \mathbb{C} : |g(x)| \leqslant 1\}$, which is well studied in numerical analysis and explicitely known for concrete schemes (see [20, p. 174—178]), does *not* contain small imaginary values.

Now we turn to concrete examples:

1) *Euler's method again:* $T_h x = x + hf(x)$.
Here $g(x) = 1 + x$ and $|g(ix)|^2 = 1 + x^2$, so $G = p = 1$.

Therefore attracting cycles occur with radius $r^2 \approx -\frac{h\omega^2}{2a}$.

This is just (2.5) for $k = 1$.

2) *Heun's method* (= *trapezoidal rule*):

$$T_h x = x + \frac{h}{2}(f(x) + f(x + hf(x))).$$

3) *Modified Euler procedure* (= *midpoint rule*):

$$T_h x = x + hf\left(x + \frac{h}{2}f(x)\right).$$

Both schemes have $g(x) = 1 + x + \frac{x^2}{2}$ and so

$$|g(ix)|^2 = \left(1 - \frac{x^2}{2}\right)^2 + x^2 = 1 + \frac{x^4}{4}.$$

Hence $p = 2$, $G = \frac{1}{4} > 0$.
Therefore attracting cycles occur with radius

$$r \approx \left(-\frac{1}{8a}\right)^{1/2} \omega^2 h^{3/2}.$$

4) *Classical Runge—Kutta-scheme:*

Here $g(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24}$ and $|g(ix)|^2 = 1 - \frac{x^6}{72} + \frac{x^8}{256}$. So $G < 0$ and our theorem does not apply. In fact there are no invariant cycles near the origin as our proof shows (if $a < 0$). The reason is that Runge—Kutta stabilizes a center, whereas the above three methods destabilize it. But of course, if we apply Runge—Kutta to a weakly unstable equation (with $a > 0$), then unstable invariant cycles of radius $r \approx \frac{\omega^3}{12a^{1/2}} h^{5/2}$ will appear which corresponds to a subcritical Hopf bifurcation.

5) *General "truncation" methods:*

Assume $g(x) = \sum_{i=0}^{k} \frac{x^i}{i!}$. It is then an easy exercise to show that $G > 0$ and hence attracting cycles occur iff k is congruent to 1 or 2 modulo 4, and $G < 0$ and hence unstable cycles occur iff k is congruent to 0 or 3

modulo 4. This is the general result which "explains" why the classical Runge—Kutta behaves different from the standard first and second order schemes treated above.

6) *Implicit Euler method:* $T_h x = x + hf(T_h x)$

Here $g(x) = \dfrac{1}{1-x}$ and $|g(ix)|^2 = \dfrac{1}{1+x^2}$, so $G = -1 < 0$.
Again we have only unstable circles.

As a general rule we can say that for any explicit RK-scheme (where g is polynomial and hence $G \neq 0$) such Hopf bifurcations arise (if $a \cdot G < 0$), either supercritical or subcritical. The only way to avoid this phenomenon would be to use those implicit methods, such as the implicit trapezoidal method $T_h x = x + \dfrac{h}{2}(f(x) + f(T_h x))$, whose growth function is a diagonal Padé-approximation of e^x. Only in this case one has $|g(ix)| \equiv 1$ and no new cycles will (should) appear.

Concluding Remarks: Somewhat related questions (perturbation of Hopf bifurcation) were treated with similar methods by IOOSS [12] and GAMBAUDO [6]. That discretization of differential equations may produce qualitatively new solutions is a wellknown phenomenon in numerical analysis. We mention only USHIKI [22], who found chaotic solutions for arbitrarily small step lengths h when applying the central difference scheme to the logistic equation.

Recently BREZZI et al. [24] have independently obtained essentially our Theorem 1 in considering the case $k = 1$ in dimension $n = 2$ for a whole Hopf family. They claim that the reduction from $\mathbb{R}^n$ to $\mathbb{R}^2$ can be done with center manifold theory. Our applications to biomathematical equations and investigations of general RK-schemes are new.

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