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BIFURCATIONS AND SPURIOUS SOLUTIONS USING NUMERICAL METHODS

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Abstract

This paper deals with bifurcations and spurious solutions using numerical methods. The mechanism by which the presence of spurious numerical solutions degrades the numerical approximation of an attractor of the underlying system in higher dimensions is studied.

1. Introduction

It is well known that a numerical method does not always produce the same asymptotic behaviour as the underlying differential equation for fixed values of the time-step. The asymptotic behaviour of a dynamical system is given by its ω-limit sets. For a numerical method to reproduce the correct asymptotic behaviour of a dynamical system, it is essential that the $\omega_{\Delta t}$-limit sets of the numerical method be close to the corresponding ω-limit sets of the differential equation. If the limit sets of the underlying system and its numerical approximation are different, then clearly so will be the dynamics of the two systems.

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The simplest ω-limit sets are fixed points. Iserles [6] showed that Runge-Kutta and linear multistep retain all the equilibria of

$$\dot{y} = f(y),\ y(0) = y_0 \in \mathbb{R}^d \tag{1.1}$$

as fixed points. However, some Runge-Kutta methods (but not linear multistep methods), may generate additional fixed points which do not correspond to equilibria of the given dynamical system. These additional fixed points are referred to as spurious fixed points and are introduced by temporal discretization studied in Iserles [6] and analyzed further in Hairer, Iserles and Sanz-Serna [4], where it was shown that any explicit Runge-Kutta method other than Forward Euler can produce spurious fixed points.

If the numerical approximation produces spurious fixed points, then the asymptotic behaviour of the numerical solution will differ from the asymptotic behaviour of the underlying system, at least for certain initial conditions. Some numerical methods including Runge-Kutta methods also admit spurious period two solutions.

Let us give an example of how a spurious solution can occur using a Runge-Kutta method

$$Y_i = y_n + \Delta t \sum_{j=1}^{s} a_{ij} f(Y_j), \tag{1.2}$$

$$y_{n+1} = y_n + \Delta t \sum_{i=1}^{s} b_i f(Y_i), \tag{1.3}$$

to approximate a differential equation. We compare the set of steady states ε of the general IVP (1.1) with the set of fixed points $\varepsilon_{\Delta t}$ of its numerical approximation.

Example 1.1. Let the differential equation

$$\dot{y} = -\rho \frac{y}{1 + y^2},\ \rho > 0, \tag{1.4}$$

be approximated by the two stage first order explicit Runge-Kutta method

$$y_{n+1} = y_n + \Delta t f(x_n, y_n). \tag{1.5}$$

The problem allows a single genuine equilibrium solution $\varepsilon = \{0\}$, whereas for the numerical method it follows that $y_{n+1} = y_n = y^*$ if

$$y^* = y^* + \Delta t f(y^* + \Delta t f(y^*)).$$

Hence

$$0 = f(y^* + \Delta t f(y^*)) = f\left(y^* - \Delta t \rho \frac{y^*}{1 + y^{*2}}\right) = -\frac{\rho y^* \left(1 - \frac{\rho \Delta t}{1 + y^{*2}}\right)}{1 + y^* \left(1 - \frac{\rho \Delta t}{1 + y^{*2}}\right)^2}$$

and

$$\varepsilon_{\Delta t} = \{0, \pm\sqrt{\rho \Delta t - 1}\} \text{ if } \Delta t > \frac{1}{\rho}, \tag{1.6}$$

where the two additional fixed points of the numerical method are spurious fixed points.

Remark. Note in Example 1.1 if we linearize about the fixed point of (1.4), then we find that $\Delta t = 1/\rho$ is the linear stability limit of the method and so the bifurcation occurs from the linear stability limit.

The linear stability function $R(z)$ as well as the set S given by

$$R(z) = 1 + zb^T (I - zA)^{-1} \boldsymbol{I}_s \tag{1.7}$$

and

$$S = \{z \in \mathbb{C} : |R(z)| \leq 1\} \tag{1.8}$$

respectively are important tools in the analysis of the so-called *spurious solutions* of (1.3) which do not correspond to solutions of the underlying system.

The spurious fixed points in Example 1.1 can be shown to be stable; thus, there will be a basin of attraction and for such initial conditions, the numerical method produces incorrect asymptotic behaviour. Moreover, since such numerical solutions are often smooth, they may not be recognized at first sight as spurious.

In general, if the spurious solutions are stable, then they may attract a large set of initial conditions, and hence the numerical approximation is no longer an "approximation" to the underlying system over long time intervals.

Furthermore, several authors [5-8] claim that unstable spurious solutions are also undesirable because the unstable manifold of the spurious solution is often connected to infinity, allowing unbounded numerical solutions and preventing the numerical solution from having an attractor. If this happens, then the structure of the underlying system will be lost. However, this claim is usually illustrated by means of one-dimensional examples. We will also illustrate this claim by considering a one-dimensional example and investigate the validity of this claim in higher dimensions by studying the Lorenz equations.

Remark. In general, if the numerical method admits spurious fixed points or period two solutions, then the ω-limit sets of the underlying system and the numerical approximation will not correspond and for certain initial conditions, the numerical solution will display false asymptotic behaviour.

In this work, we will study the mechanism by which the presence of spurious numerical solutions degrades the numerical approximation of an attractor of the underlying system. We consider a one-dimensional example, where it is shown that the unstable manifold of the spurious solution is connected to infinity, thus allowing unbounded numerical solutions and preventing the numerical solution from having an attractor.

We will then extend our analysis to a three-dimensional problem. This will provide the basis for our study of the mechanism by which spurious solutions generated by Runge-Kutta methods and which bifurcates at the linear stability limit result in the destruction of the attractor. In particular, we study the behaviour of the numerical approximation generated by an explicit second order Runge-Kutta method to the Lorenz equations

$$\begin{cases} \dot{x} = \sigma(y - x) \\ \dot{y} = rx - y - xz \\ \dot{z} = xy - bz \end{cases} \tag{1.9}$$

with parameter values chosen such that $\sigma = 10$, $b = 8/3$. Initially, we consider the case $r = 8$. We will show that for step-sizes close to the linear stability limit, the unstable manifold of the spurious fixed point is not connected to infinity. However, for larger step-sizes, this unstable manifold is connected to infinity and there are numerical solutions in an unstable manifold of the origin which go close to the spurious solution and then follow its unstable manifold to infinity. Hence, the presence of a spurious solution with its unstable manifold connected to infinity destroys the numerical attractor.

2. Fixed Point Bifurcation for a Runge-Kutta Method

Often spurious solutions bifurcate from the linear stability limit (see Example 2.1 and [1, 2]). This should not be a surprise since a stable fixed point loses its stability at the linear stability limit and we should expect bifurcation to occur. It should be noted that spurious solutions can persist for arbitrarily small step-sizes Δt and hence incorrect asymptotic behaviour of the dynamical system can occur at step-sizes used in practical implementation.

We are interested in the mechanism by which the presence of spurious numerical solutions degrades the numerical approximation to an attractor of the underlying system.

Example 2.1. Consider the initial value problem

$$\dot{y} = -(y + y^3), \; y(0) \in \mathbb{R}, \tag{2.1}$$

where a numerical approximation is obtained using the Runge's second order method

$$\begin{cases} k_1 = \Delta t f(x_n, y_n), \\ k_2 = \Delta t f\left(x_n + \frac{1}{2}\Delta t,\ y_n + \frac{1}{2}k_1\right), \\ y_{n+1} = y_n + k_2 + O(\Delta t^3). \end{cases} \tag{2.2}$$

From (2.2) for a fixed point of the Runge's method

$$f(Y_2) = 0. \tag{2.3}$$

Thus, if $y_n = y_{n+1}$ is a fixed point of the numerical method (2.2), then Y_2 is a fixed point of the dynamical system (2.1). One possibility is that $y_n = y_{n+1} = Y_2$, however, it is also possible for spurious fixed points to occur as we will now demonstrate. The origin is the only fixed point of (2.1), $\varepsilon = \{0\}$, since $f(0) = 0$, and f is strictly monotonic in y. Thus, $f(Y_2) = 0$, if and only if $Y_2 = 0$. Hence, if the numerical approximation (2.2) admits a spurious solution with $y_n = y_{n+1} = y^*$, then we must have $Y_2 = 0$ and hence

$$0 = Y_2 = y^* + \frac{\Delta t}{2} f(y^*) = y^*\left[1 - \frac{\Delta t}{2}(1 + y^{*^2})\right]$$

which yields

$$\varepsilon_{\Delta t} = \left\{y^* = 0 \text{ or } y^{*^2} = -1 + \frac{2}{\Delta t},\ \Delta t < 2\right\}.$$

Now, $y^* = 0$ is not a surprise because 0 is also a fixed point of the dynamical system (2.1), so must be a fixed point for the method. For $y^{*^2} = -1 + 2/\Delta t$, we obtain the solution we have already if $\Delta t = 2$. Bifurcation occurs at this step-size, where spurious solutions bifurcate from the trivial solution and for $\Delta t < 2$ yields additional spurious solutions. In this example, the bifurcation where the spurious solution bifurcates is known as a *pitchfork bifurcation* (see [9]) because of the shape of the graph, e.g., Figure 1. In Figure 1, the set of fixed points and spurious fixed point solutions for the initial value problem (2.1) are plotted. As $\Delta t \to 0$, then the spurious solution tends to infinity.

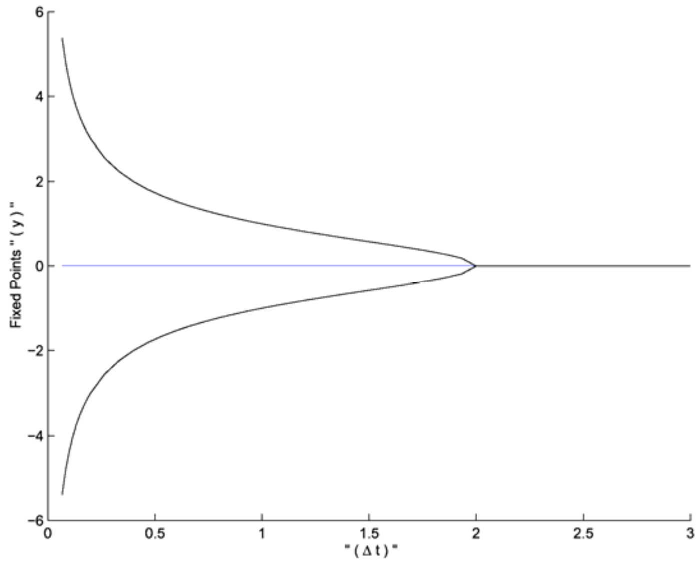

Figure 1. Spurious solutions for the one dimensional Problem (2.1).

Note that in Example 2.1, spurious solutions are generated in spurious bifurcations at the linear stability limit of the numerical method at the genuine fixed point. In general, as in the example, these spurious solutions may exist for Δt arbitrarily small but as $\Delta t \to 0$ they become unbounded (see [5] for further details and the references therein).

Now, we consider a three-dimensional problem. Let the Lorenz equations be defined by (1.9), and let us investigate the behaviour of the numerical approximation generated again by an explicit second order Runge-Kutta method given by (2.2). The parameter values are chosen such that $\sigma = 10$, $b = 8/3$ and initially we will consider $r = 8$. With this choice of parameters, the fixed points of the system given by

$$\varepsilon = \{\varepsilon^0 := (0, 0, 0),\ \varepsilon^{+/-} := (\pm\sqrt{b(r-1)}, \pm\sqrt{b(r-1)}, r-1)\}$$

are

$$\varepsilon = \left\{(0, 0, 0), \left(\sqrt{\frac{56}{3}}, \sqrt{\frac{56}{3}}, 7\right), \left(-\sqrt{\frac{56}{3}}, -\sqrt{\frac{56}{3}}, 7\right)\right\}$$

and linearising (1.9) about the origin, we obtain the following eigenvalues with the corresponding eigenvectors as calculated in MATLAB

$$\lambda_1 = 4.512, \quad v_1 = (-0.567 \quad -0.823 \quad 0)^T,$$
$$\lambda_2 = -2.667, \quad v_2 = (0 \quad 0 \quad 1)^T,$$
$$\lambda_3 = -15.512, \quad v_3 = (-0.876 \quad 0.483 \quad 0)^T. \tag{2.4}$$

Spurious fixed points will bifurcate from the origin at the linear stability limit in each of the directions corresponding to a negative eigenvalue. Since $\lambda_3 < \lambda_2 < 0$, the bifurcation in the v_3 direction occurs at a smaller step-size $(\Delta t = -2/\lambda_3 \simeq 0.12892)$ than the v_2 bifurcation $(\Delta t = -2/\lambda_2 \simeq 0.44321)$, hence it is the λ_3 bifurcation in which we will be interested.

For Runge's method (2.2) at a fixed point, we have $y_{n+1} = y_n$ and so (2.3) is satisfied. Hence, Y_2 must be a fixed point of the dynamical system. Thus, if y_n is a fixed point of Runge's method, then

$$Y_2 = y_n + \frac{\Delta t}{2} f(y_n),$$

where Y_2 is a fixed point of the dynamical system.

Now, we are interested in the branch of spurious solutions which bifurcate from the origin at the linear stability limit. At the linear stability limit, the spurious fixed point coincides with the fixed point of the dynamical system and so $y_n = y_{n+1} = Y_1 = Y_2 = (0, 0, 0)$. As we follow this branch of spurious solutions by varying Δt, $y_n = y_{n+1} = Y_1$ will vary continuously with Δt. But, since $Y_2 = (0, 0, 0)$ at the bifurcation point and by (2.3), $f(Y_2) = 0$ for all Δt, it follows that $Y_2 = (0, 0, 0)$ for all Δt, since $(0, 0, 0)$ is an isolated fixed point of the dynamical system. Thus, if $y^* = (y_1^*, y_2^*, y_3^*)$ is a fixed point of (2.2), then

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} y_1^* \\ y_2^* \\ y_3^* \end{pmatrix} + \frac{\Delta t}{2} f \begin{pmatrix} y_1^* \\ y_2^* \\ y_3^* \end{pmatrix} \Rightarrow \begin{cases} y_1^* + 5\Delta t(y_2^* - y_1^*) = 0 \\ y_2^* + \dfrac{\Delta t}{2}(8y_1^* - y_2^* - y_1^* y_3^*) = 0 \\ y_3^* + \dfrac{\Delta t}{2}(y_1^* y_2^* - 8/3\, y_3^*) = 0 \end{cases}$$

and

$$\begin{cases} y_1^*(\Delta t) = \pm \dfrac{5\sqrt{6}\Delta t}{15\Delta t^2(1-5\Delta t)} \sqrt{(35\Delta t^2 + 11\Delta t - 2)(20\Delta t^2 - 19\Delta t + 3)} \\ y_2^*(\Delta t) = \pm \dfrac{\sqrt{6}}{15\Delta t^2} \sqrt{(35\Delta t^2 + 11\Delta t - 2)(20\Delta t^2 - 19\Delta t + 3)} \\ y_3^*(\Delta t) = \dfrac{35\Delta t^2 + 11\Delta t - 2}{5\Delta t^2}. \end{cases} \tag{2.5}$$

Since we are looking for bifurcations at the origin, then at $\Delta t = -11/70 + \sqrt{401}/70 \approx 0.1289$ $(y_1^*, y_2^*, y_3^*) = (0, 0, 0)$ and we obtain a spurious fixed point which bifurcates from the origin. Note that these solutions exist only for $\Delta t \geq -11/70 + \sqrt{401}/70$, since for $\Delta t < -11/70 + \sqrt{401}/70$, then $35\Delta t^2 + 11\Delta t - 2 < 0$. Finally, it should also be noted that as $\Delta t \to 1/5$, $y_1^*(\Delta t) \to \infty$ and so the spurious solution becomes unbounded.

3. Numerical Investigation of the Effect of the Spurious Solution on a Numerical Method

In this section, we present some numerical simulations. These results provide the basis for a study of the mechanism by which the spurious solutions generated using Runge's method (2.2) and which bifurcate at the linear stability limit result in the destruction of the attractor. We are particularly interested in whether the unstable manifold of the spurious solutions are unbounded and whether this destroys the numerical attractors.

We will see that a numerical approximation to the attractor persists for step-sizes above the linear stability limit at which the spurious fixed points exist, because the unstable manifolds of these spurious fixed points are connected to the genuine non-zero fixed points of the Lorenz equations (1.9). However, for larger step-sizes, the unstable manifolds of the spurious solutions are connected to infinity as is the (numerical) unstable manifolds of the fixed point at the origin. Thus, there is no numerical attractor.

Note that there is a one-dimensional unstable manifold at the origin for the Lorenz equations (1.9), and if we use a step-size larger than the bifurcation point ($\Delta t > 0.1289$), the numerical approximation has a two-dimensional unstable manifold, whose linear unstable manifold is the span of v_1 (the linear unstable manifold of the origin for the Lorenz equations) and v_3 (which becomes unstable in the bifurcation at the linear stability limit) and hence is a plane (see [3]).

We use Runge's method (2.2) with step-sizes $\Delta t = 0.13, 0.132, 0.146$ and initial condition

$$y_0 = \varepsilon(v_1(\cos\theta) + v_3(\sin\theta)), \tag{3.1}$$

where v_1 and v_3 are the eigenvectors defined in (2.4). Provided we multiply (3.1) by a small number ε, then we are close to the origin, hence the linear unstable manifold is close to the actual unstable manifold. Therefore, the initial conditions considered are close to the numerical unstable manifold of the origin.

Now, using MATLAB in Figure 2(i) for step-size $\Delta t = 0.13$, the spurious solutions are represented by the two circles and the unstable manifold of one of the spurious fixed points are plotted as dash dotted line. In both directions, the unstable manifolds of the spurious fixed point converge to the two non-zero genuine fixed points of the Lorenz equations (1.9).

Next, we consider orbits of the numerical unstable manifold of the origin (dotted and solid lines). For initial condition close to the origin, in the direction of the v_1 eigenvector which is in the linear unstable manifold of the origin for the Lorenz equations and also in the linear unstable manifold for its numerical approximation, the numerical solution (dotted line) converges to the genuine non-zero fixed points of the Lorenz equations. Furthermore, taking an initial condition in the direction of the v_3 eigenvector which is in the linear stable manifold of the origin for the Lorenz equations (1.9) but which is in the linear unstable manifold for its numerical approximation, we see that the numerical solution (solid line) also converges to the genuine non-zero fixed points and it does not provide a chaotic behaviour; moreover, this solution remains close to the previous solution throughout.

In Figure 2(ii), the spurious solutions for a slightly larger step-size $\Delta t = 0.132$ are represented again by the two circles, and the unstable manifolds of one of the spurious fixed points are plotted as dash dotted line in the graph. In one direction, the part of the unstable manifold travelling to the right at the spurious solution on the graph converges to the right hand non-zero fixed point. The unstable manifold travelling to the left of the spurious solution passes relatively close to the other non-zero genuine fixed point but then its x and y coordinate change sign and it converges to the same non-zero genuine fixed point as the other half.

Now, let us consider the numerical unstable manifold at the origin (dotted and solid lines). Note that the numerical unstable manifold from the origin is a two-dimensional set. As before, for initial conditions close to the origin in the direction of the v_1 eigenvector, we see similar behaviour as to the case of $\Delta t = 0.13$; that the numerical solution (dotted line) is similar to the exact solution of the Lorenz equations and converge to a genuine non-zero fixed point. However, for initial conditions close to the origin in the direction of the v_3 eigenvector which is in the linear stable manifold of the origin for the dynamical system (1.9) but which is in the linear unstable manifold for its numerical approximation, the numerical solution (solid line) goes far away from the origin, and rather than converging to the non-zero fixed point on the side of the origin to which it initially travels, the x, y variables actually change sign and the numerical solution converges to the other genuine non-zero fixed point of the Lorenz equations.

Finally, in Figure 2(iii), we increase the step-size again $\Delta t = 0.146$. The spurious solutions are represented by the two circles, and the unstable manifold of one of the spurious fixed points are plotted as dash dotted line in the graph. In one direction, the part of the unstable manifold travelling to the right at the spurious solution on the graph converges to the right hand non-zero fixed point. However, the unstable manifold travelling to the left of the spurious solution becomes unbounded.

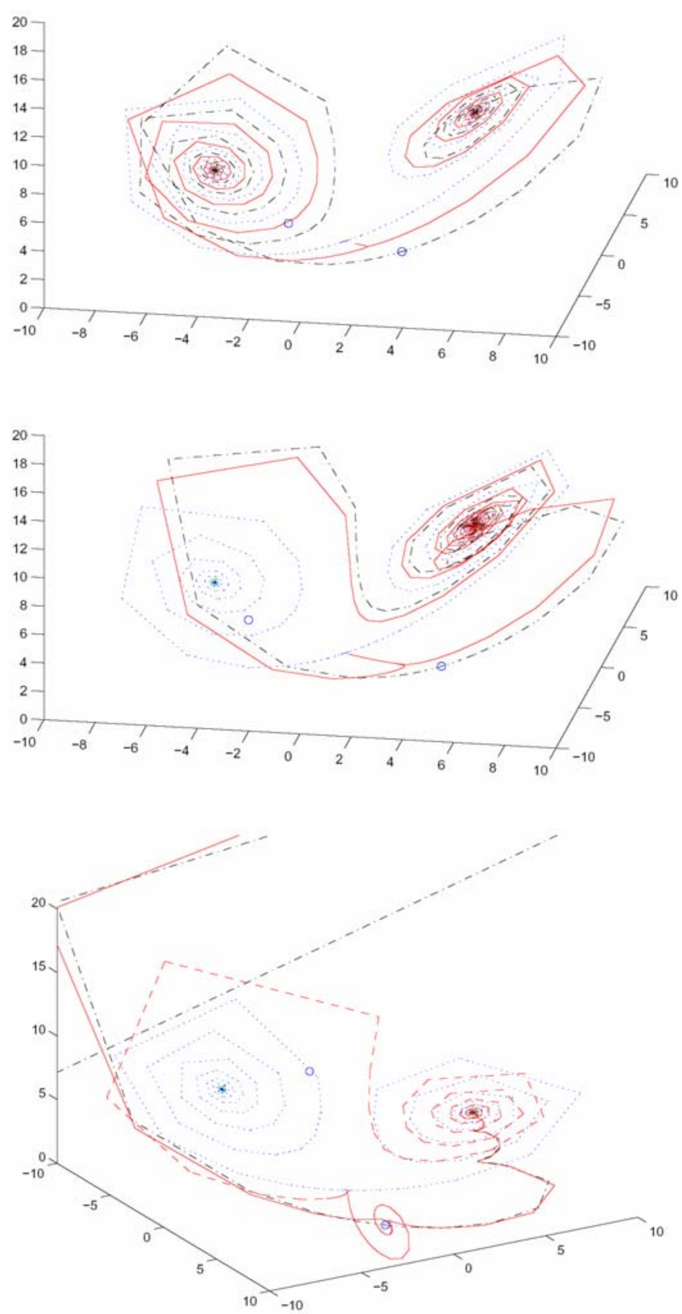

Figure 2. Numerical simulation of the Lorenz equations with (i) $\Delta t = 0.13$, (ii) $\Delta t = 0.132$ and (iii) $\Delta t = 0.146$.

Now, we consider the numerical unstable manifold at the origin (dotted and solid lines). As before, for initial conditions close to the origin in the direction of the v_1 eigenvector, we see similar behaviour as to the case of $\Delta t = 0.13$ and $\Delta t = 0.132$; that the numerical solution (dotted line) is similar to the exact solution of the Lorenz equations and converge to a genuine non-zero fixed point. Then for initial condition close to the origin and close to the direction of the v_3 eigenvector which is in the linear stable manifold of the origin for the dynamical system (1.9) but which is in the linear unstable manifold for its numerical approximation, we find numerical solutions (solid lines) which go close to the spurious fixed point in such a way that the spurious fixed point becomes a saddle focus. Then follow its unstable manifold of the spurious fixed point in either directions. Thus, if we start near the fixed point at the origin, we get orbits that tend to infinity at the same time as the dynamics from the spurious solution does.

4. Conclusion

We investigated the mechanism by which the presence of spurious numerical solutions degrades the numerical approximation of an attractor of the underlying system. In particular, we studied the behaviour of the numerical approximation generated by an explicit second order Runge-Kutta method to the Lorenz equations (1.9) with parameter values chosen such that $\sigma = 10, b = 8/3$ and initially will consider $r = 8$.

We have seen that the spurious solution bifurcates at a certain step-size $\Delta t \approx 0.1289$. Above that step-size and close to it, we see the numerical solution is not greatly affected by the presence of the spurious solution. Then the numerical attractor is destroyed in a secondary bifurcation at which the unstable manifold of the spurious solution is connected to infinity. Hence, there are numerical solutions in the unstable manifold of the origin which pass close to the spurious solution and then follow its unstable manifold to infinity. So, the presence of a spurious solution with its unstable manifold connected to infinity destroys the numerical attractor, although there is a range of step-size values close to the linear stability limit for which we have the presence of a spurious solution but we still have a numerical attractor.

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