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Discrete-time and continuous-time modelling: some bridges and gaps

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The relationship between continuous-time dynamics and the corresponding discrete schemes, and its generally limited validity, is an important and widely acknowledged field within numerical analysis. In this paper, we propose another, more physical, viewpoint on this topic in order to understand the possible failure of discretisation procedures and the way to fix it. Three basic examples, the logistic equation, the Lotka–Volterra predator–prey model and Newton's law for planetary motion, are worked out. They illustrate the deep difference between continuous-time evolutions and discrete-time mappings, hence shedding some light on the more general duality between continuous descriptions of natural phenomena and discrete numerical computations.

1. Introduction

This special issue of *Mathematical Structures in Computer Science* is devoted to the ubiquitous duality between discreteness and continuity, and to the debates that have arisen with the aim of reconciling or contrasting these two notions. We shall consider this issue within a more restricted scope – throughout this paper we will use 'continuous' and 'discrete' to mean continuous or discrete in *time*, and with reference to the modality used to describe a *deterministic* evolution: either by a continuous trajectory $t \in [0, \infty[\to x(t)$, or as a discrete sequence $(x_n)_n$ labelled by integers. Our main aim is to give a simple and comprehensive account of results scattered in the literature.

A striking difference between discrete and continuous modellings, which is further explained in Section 2, is related to the *occurrence of deterministic chaos*, namely, the seemingly erratic behaviour originating in nonlinear amplification of any perturbation (sensitivity to initial conditions) and the mixing of phase space regions. Discrete autonomous dynamical systems in 1-dimension can exhibit chaotic behaviour, whereas the corresponding (1-dimensional) continuous evolution equations rule it out, and cannot even possess a nontrivial periodic solution. A phase-space dimension $d \geqslant 3$ is required to observe (possibly) a chaotic behaviour in a continuous dynamical system (see, for instance, the textbook Devaney (1989)). This point suggests that the passage from discrete to continuous equations, or the converse, is anything but insignificant. Moreover, we cannot avoid this issue since any numerical resolution of a continuous equation does, in fact, *imply a recourse to a discrete analogue*: it is thus of the utmost importance for us to describe the relationship between the desired (continuous) solution and the output of the actual (discrete) computation.

In Section 2, we present some caveats concerning the passage from discrete to continuous equations, and conversely, on the paradigmatic Verhulst logistic equation, investigating, in particular, the status and influence of the actual size of the *unit time step* in discrete modellings, and providing a physical interpretation of standard numerical analysis procedures. In Section 3, we consider a 2-dimensional evolution, which brings new difficulties, though some guidelines can be laid down in the case of Hamiltonian systems, based on their symplectic structure. We recall in Section 4 the historical example of Newton's derivation of Kepler's law. Finally, in Section 5 we draw some general conclusions enlarging the scope of the three case studies.

2. From discrete to continuous dynamics and back: How large is 1?

2.1. *The discrete-time logistic evolution*

The logistic map $f_a(x) = ax(1-x)$ giving the celebrated recursion relation on the interval $[0, 1]$

$$x_{n+1} = ax_n(1 - x_n) = f_a(x_n) \qquad x_0 \in [0, 1] \quad a \in]1, 4] \tag{1}$$

is one of the simplest example of *discrete autonomous evolution leading to chaos.* This nonlinear equation was introduced by Verhulst (a Belgian mathematician) in 1838 to take into account the fact that a, the Malthus coefficient characterising the growth of the population

$$X_{n+1} = aX_n,$$

has to decrease when X_n increases, due to the limitation of resources (Verhulst 1838). The simplest way was to replace the constant rate a by a linear dependence in X_n, matching the rate a at vanishing population, namely $a(1-X_n/M)$; the parameter M is then interpreted as being the maximum acceptable population, currently known as the 'carrying capacity' of the environment. Equation (1) is recovered by substituting $x_n = X_n/M$. A very rich variety of dynamic behaviours is generated by Equation (1), whose temporal structure is governed by the values of the control parameter a. Since the seminal reference† (May 1976), several studies of the asymptotic dynamics of (1) have been published, amongst which Evans and Morriss (1991), Peitgen *et al.* (1992) and Korsch and Jodl (1998) are very pedagogical. Here, we will just review the most significant properties.

For a given, such that $1 < a < a_1 = 3$, the fixed point $x_a^* = 1 - 1/a$ is stable and globally attractive, therefore $x_n \to x_a^*$ as $n \to \infty$, irrespective of the initial condition x_0, provided it lies within its basin of attraction $]0, 1[$. If $a_1 = 3$, a cycle of period 2 appears through a pitchfork bifurcation. This is also called a period-doubling bifurcation

† Without wishing to denigrate the historical importance and repercussions of this paper, one should note that rather more is known today about the asymptotic behaviour in the region $a > a_\infty$, and this leads us to modify May's claim that all trajectories are periodic but with period so large that the dynamics resembles chaos.

since it is associated with the destabilisation of a fixed point x_a^* into a 2-cycle (or the destabilisation of a 2^n-cycle into a 2^{n+1}-cycle when it involves $f_a^{2^n}$ rather than f_a), and this generic bifurcation is characterised by the relation $f'_{a_1}(x^*_{a_1}) \equiv \partial_x f(a_1, x^*_{a_1}) = -1$ and the generic condition $\partial^2_{ax} f(a_1, x^*_{a_1}) \neq 0$, where, for clarity, we have denoted the a-dependence on the same footing (Iooss and Joseph 1981). The 2-cycle emerging in a_1 remains stable and globally attractive in $]0,1[$ for any $3 < a < a_2 = 1 + \sqrt{6}$. More generally, there exists an increasing sequence $(a_k)_k$ of bifurcation values such that for $a_k < a < a_{k+1}$, the asymptotic regime is a cycle of period 2^k, which destabilises in a_{k+1} through a pitchfork bifurcation of $f_a^{2^k}$. This sequence converges to $a_\infty \approx 3.5699$ according to the scaling law $a_\infty - a_k \sim \delta^{-k}$ with a *universal* rate $\delta \approx 4.6692$ (Feigenbaum 1978; Coullet and Tresser 1978). The discrete evolution given by Equation (1) is actually a generic example exhibiting this so-called period-doubling scenario toward chaos, that is, a normal form to which any one-parameter family experiencing such a scenario is conjugated (Collet and Eckmann 1981). If $a = a_\infty$, a chaotic behaviour arises, which is reflected for $a > a_\infty$ in a positive Lyapunov exponent (sensitivity to initial conditions) and mixing property (time decorrelation of phase space regions). Chaotic regions in the a-space then intermingle in a highly complicated fashion (though this is now understood (Collet and Eckmann 1981)) with non-chaotic regions where stable odd cycles rule the asymptotic dynamics.

The conclusion is now accepted, but was striking when May (1976) was published: a large variety of chaotic behaviours can be generated by a 1-dimensional *discrete* evolution, with a seemingly harmless nonlinearity (smooth and simply quadratic). The results recalled above showed unquestionably that nonlinearities are never harmless when supplemented by a folding dynamics, here coming from the bell shape of the evolution map. But the role and importance of the time-discrete nature of the evolution rule are far less clear, and we shall pursue the analysis further in this direction.

2.2. *Continuous-time counterpart: a trivial dynamics*

As it is impossible to give an analytic solution† of (1), that is, x_n as an explicit function of n and x_0, and because we are interested in the asymptotic solution $n \to \infty$ (which gives a vanishing relative duration to the unit step $n \to n+1$), it is appealing to deal with the corresponding continuous problem (Hubbard and West 1991), which is straightforwardly solvable. To derive a continuous counterpart of (1), one subtracts x_n from both sides of Equation (1) and identifies $x_{n+1} - x_n$ with the differential of a continuous function of time $y(t)$, which leads to

$$\frac{dy}{dt} = f_a(y) - y = y[a(1-y) - 1], \tag{2}$$

whose analytic solution is easily obtained as

$$y(t) = \frac{(a-1)y_0}{ay_0 + [a(1-y_0) - 1]e^{-(a-1)t}}. \tag{3}$$

† Except for when $a = 4$, where $x_n = \sin^2(2\pi\theta_n)$ with $\theta_n = 2\theta_{n-1} = 2^n\theta_0$ if $x_0 = \sin^2(2\pi\theta_0)$. This equivalence with the angle-doubling $\theta_{n+1} = 2\theta_n$ (modulo 1) allows us to prove that one gets a fully chaotic behaviour for $a = 4$ (the location of x_n below 1/2, coded 0, or above 1/2, coded 1, generates a binary sequence that is statistically equivalent to the outcome of a game of heads-and-tails).

This solution is obviously regular with respect to $t \geqslant 0$ for any value of $a > 1$ and, not surprisingly, tends to x_a^* as $t \to \infty$. In contrast with this simple behaviour, which is qualitatively insensitive to the value of $a > 1$, any attempt to solve (2) by discretisation with a time step $h = 1$ will lead to the logistic evolution (1) with its full richness of solutions as a is varied. On the other hand, one expects that, for h small enough, one should approach the true solution (3). To see how this is possible, we have to quantify what we mean by '*small enough*'.

2.3. *Interpretation of discretisation schemes associated with the logistic equation*

In this section we will recall the behaviour of the discretisation schemes associated with Equation (2) (Borrelli and Coleman 1998). Our aim is not to produce new results for this equation, or to devise an accurate numerical resolution, but rather to understand in this tractable and well-understood situation what can currently be done to solve real problems when no straightforward solution is available. For a given time step h, the discretisation scheme is given by

$$y(t+h) = y(t) + h\{ay(t)\,[1 - y(t)] - y(t)\}. \tag{4}$$

A remarkable feature of the logistic equation is the possibility of rewriting this scheme as

$$Y(t+h) = AY(t)\,(1 - Y(t)), \tag{5}$$

with

$$Y(t) = \lambda y(t) \quad \text{where} \quad \lambda = \frac{ah}{1 + h(a-1)}, \tag{6}$$

involving the effective control parameter

$$A(a, h) = 1 + h(a-1) \tag{7}$$

provided $y_0 \in [0, 1/\lambda]$ (note that $\lambda < 1$ if $h < 1$). Obviously, the same phenomenology as we get for the evolution given by Equation (1) will be observed. For instance, the inequality $A < a_1 = 3$, required to obtain the convergence of (5) to the nontrivial fixed point $Y_A^* = 1 - 1/A$, means

$$h < h_c(a) = \frac{a_1 - 1}{a - 1} = \frac{2}{a - 1}. \tag{8}$$

Extending the reasoning to the subsequent bifurcations, one would observe the whole period-doubling scenario when the discretisation step h increases, namely, at values $(h_k)_k$ with $A(a, h_k) = a_k$, that is,

$$h_k = \frac{a_k - 1}{a - 1}. \tag{9}$$

Chaos occurs for $h > h_\infty(a) = (a_\infty - 1)/(a-1)$. The bifurcation diagram as a function of h, at fixed a, would then be similar to the standard bifurcation diagram in a-space, up to a rescaling of the attracting sets by a factor of $\lambda(a, h)$, a translation and a rescaling of the bifurcation values ($a_k = 1 + (a-1)h_k$). In particular, it is interesting to note that the

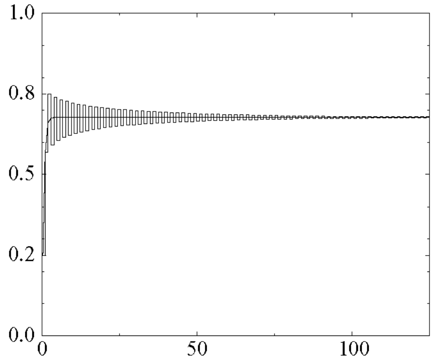

Fig. 1. Discretisation of the logistic equation (2) with $a = 3.1$, using a time step $h < h_c$ (here $h = 0.94$, while $h_c \equiv 2/(a-1) = 20/21 \approx 0.95$), see text, Section 2.3. The bold line shows the exact (continuous-time) solution of (2). Stair step $\frac{1}{\lambda} f_A(nh)$. $x_a^* = 1 - 1/a$. The behaviour near the origin is shown in the inset.

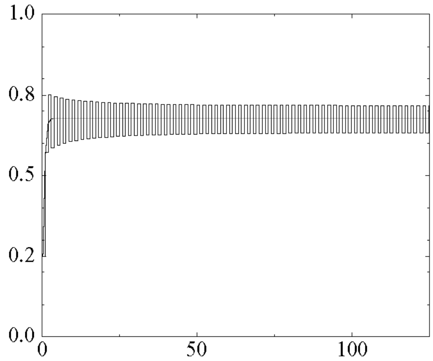

Fig. 2. This is the same as Figure 1 but with $h = 0.96 > h_c$.

sequence $(h_k)_k$ follows the same universal scaling law $h_\infty - h_k \sim \delta^{-k}$, or, more precisely,

$$\frac{h_{i+1} - h_i}{h_{i+2} - h_{i+1}} \longrightarrow \delta \quad \text{when} \quad i \to \infty \quad \text{with} \quad \delta \approx 4.4669. \tag{10}$$

As an example, consider the case $a = 3.1$ (Figures 1, 2 and 3). The critical value of h is $h_c = (a_1 - 1)/(a - 1) = 2/2.1 \simeq 0.9524$. For $h > h_c$, one gets a 2-cycle, namely oscillations of the solution between the two (stable) fixed points of $f_A[f_A(Y)]$. The onset of chaos occurs for $h = h_\infty = (a_\infty - 1)/(a - 1) = 2.5699/2.1 = 1.22376$.

2.4. *Discussion: an interplay between two characteristic times*

This simple study illustrates that the passage from continuous-time to discrete-time in a nonlinear evolution is not insignificant: an actual chaotic behaviour can be suppressed by replacing a discrete model by its limiting continuous counterpart, or, conversely, destabilisation of the continuous-time evolution, leading to cycles and even a spurious

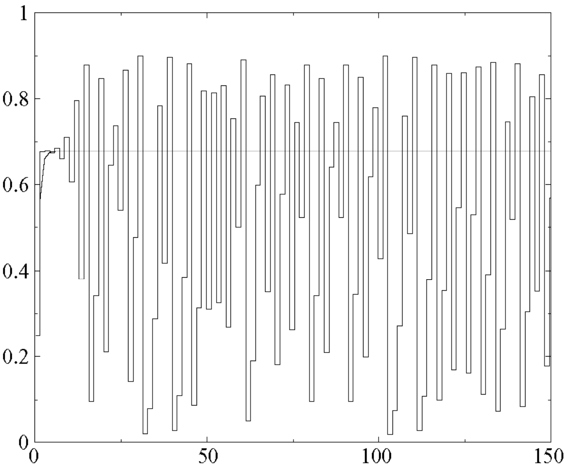

Fig. 3. Discretisation of the logistic equation (2) with $a = 3.1$, using a time step $h = 3/(a-1) = 1.424$ corresponding to the fully chaotic case $A = 4$, see text, Section 2.3.

chaotic behaviour, might follow from an improper choice of the discretisation step (Yamaguti and Matano 1979).

However, the passage from Equation (1) to (5) by a simple scaling is exact only in the case of the quadratic family. To enlarge the scope of our discussion, we shall now investigate what can be carried over to more general situations. Let f be a map, generating a discrete dynamical system $x_{n+1} = f(x_n)$ and having a stable fixed point x^* (that is, $f(x^*) = x^*$ and $|f'(x^*)| < 1$). The naive continuous counterpart is given by $dy/dt = f(y) - y$. Linear stability analysis shows that x^* is still (at least locally) a stable fixed point of the continuous dynamics since the linear growth rate of perturbations is negative: $f'(x^*) - 1 < 0$.

We might then consider the discrete scheme $z_{n+1} = z_n + h[f(z_n) - z_n]$ for various values of the time step h. It is straightforward to show that this discretisation scheme destabilises for $h > h_c$ where

$$h_c = 2/[1 - f'(x^*)]. \tag{11}$$

Indeed, the linear stability of x^* breaks down when the modulus $|1 + h(f'(x^*) - 1)|$ overwhelms 1, which occurs for $1 + h(f'(x^*) - 1) = -1$. This relation yields the above value of h_c and shows that the discrete scheme exhibits a period-doubling (pitchfork) bifurcation in $h = h_c$ (one can check directly that the additional generic condition for this bifurcation stated in Section 2.1 is also fulfilled).

The additional feature observed when the map f_a depends on a control parameter a and exhibits a period-doubling in a_1 is that $h_c(a)$ crosses $h = 1$ in $a = a_1$: for $a > a_1$, $f'_a(x^*_a) < -1$ and x^*_a is unstable with respect to the initial discrete dynamics ($h = 1$) but is still a stable fixed point of the continuous dynamics, showing the inadequacy of the limiting continuous model $dy/dt = f_a(y) - y$ for capturing the behaviour of the discrete one $x_{n+1} = f_a(x_n)$. Note that, in the case when $f'_a(x^*_a)$ decreases with a (as in the logistic example), $h_c(a)$ decreases if a increases: as the fixed point becomes more stable (that is,

$|f'_a(x^*_a) - 1|$ becomes larger with $f'_a(x^*_a) - 1 < 0$), the time-step range of validity of the discretisation scheme becomes smaller (in a sense, the discretisation scheme becomes less stable).

The qualitative differences between the continuous-time and discrete-time versions of the logistic equation (which were described explicitly in earlier sections, and above in a more general framework) are not really surprising: a general claim asserts that a continuous-time dynamics requires a phase space of dimension at least 3 to develop chaotic behaviour (Schuster 1984). In dimension 1 or 2, continuous trajectories behave as mutual boundaries for each other (trajectories of an autonomous continuous dynamic system cannot cross each other), which obviously prevents chaos (and even nontrivial periodic solutions in dimension 1). But, while it is straightforward to foresee the loss of chaotic and even periodic behaviour when turning to the limiting continuous dynamics, one may ask if it is possible to understand on physical grounds the existence of a critical value h_c for the discretisation time step h.

The explanation lies in a comparison of the intrinsic time scale(s) of the dynamics with the chosen 'time unit' h. The characteristic time of a continuous evolution, which we will continue to denote by $dy/dt = f(y) - y$ to avoid a proliferation of new notation, can be estimated as $\tau \sim 1/[1 - f'(x^*)]$. Indeed, a mere linearisation of (2) around the fixed point x^* leads to

$$\frac{d}{dt}[x(t) - x^*] = [f'(x^*) - 1](x - x^*), \tag{12}$$

whose solution is $x(t) - x^* \sim e^{-t[1-f'(x^*)]}$, and hence the value of τ. The discretisation scheme is destabilised when $h > h_c = 2\tau$. The stepwise updating, after each time step h, of the evolution law is too rough to control the discrete evolution properly and to force it to follow closely all the relevant variations of the continuous trajectory.

This is reminiscent of the *Nyquist theorem* (Nyquist 1928; Shannon 1949) for a periodic continuous evolution: the observation time step should be smaller than half the smallest period (or characteristic time) to sample the continuous trajectory properly.

Note that τ or, equivalently, the critical value $h_c = 2\tau$ of the time step are intrinsic features of the dynamics, in the sense that they are invariant through conjugacy. This means that for any diffeomorphism ϕ, we have that f and $\phi^{-1} \circ f \circ \phi$ (which provides an equivalent modelling of the discrete model associated with f) have the same critical value h_c and the same characteristic time τ. Indeed, if we use $y^* = \phi^{-1}(x^*)$ to denote the fixed point of $\phi^{-1} \circ f \circ \phi$, it is easy to check that $f'(x^*) = [\phi^{-1} \circ f \circ \phi]'(y^*)$, from which we get the equality of the characteristic times associated with f and $\phi^{-1} \circ f \circ \phi$, respectively.

We will now pursue the comparison between the continuous evolution and its discretisation a little further in order to understand the emergence of oscillations for $h > 2\tau$. The general continuous equation $dy/dt = f(y) - y$ operates a fine tuning of the evolution rate dy/dt that is obviously not achieved by updating $f(y) - y$ at times $t_n = nh$. We have shown here that, near a stable fixed point, the resulting discrepancies lead to a bifurcation in the asymptotic dynamics when h overwhelms the characteristic time of the evolution. To take a familiar example of such oscillations arising from a mismatch between two characteristic times, consider a heating/cooling device that is able to measure the difference between the instantaneous room temperature and a prescribed one, and adjust the appropriate energy supply or extraction to counteract the measured difference. If the time h necessary for the device to actually deliver the required energy is longer than the characteristic time of temperature variations in the environment, the device will not balance the external temperature variations but rather, its ill-phased response will dominate, and the room temperature will suffer large oscillations. More generally, *any ill-tuned homeostatic device, responding with a large time lag h, will produce oscillations*, and the result of Section 2.3 is the mathematical translation of this ubiquitous phenomenon.

2.5. *Generalised Euler discretisation schemes*

In fact, the improvement in the validity range of a discretisation scheme given by using an implicit recursion relation is a general property. In particular, one can check that the implicit scheme

$$x_{n+1} = x_n + h[ax_{n+1}(1 - x_{n+1}) - x_{n+1}] \tag{13}$$

(with the notation $x_n \equiv x(t_n)$ where $t_n = t_0 + nh$) for the logistic equation is stable for arbitrarily large time steps h (Hubbard and West 1991).

As an illustration of the general ideas, consider the simpler case of a 1-dimensional dynamical system $dx/dt = g(x)$ having a stable fixed point x^*, that is, $g(x^*) = 0$ and $g'(x^*) < 0$. The first-order Euler scheme $z_{n+1} = z_n + hg(z_n)$ destabilises in $h_c = 2/|g'(x^*)|$ through a pitchfork bifurcation (see Section 2). Higher-order schemes are given by

$$\begin{aligned} z_{n+1} &= F_q(h, z_n) \equiv z_n + hg(z_n) + \frac{h^2}{2} g(z_n)g'(z_n) \\ &\quad + \frac{h^3}{6}([g(z_n)]^2 g''(z_n) + g(z)[g'(z_n)]^2) + \cdots + h^q G_q(z_n). \end{aligned} \tag{14}$$

Direct computation of $\partial_x F_q(h, x^*)$ yields the following results:

- The second-order scheme ($q = 2$) destabilises at the same value $h_{c,2} = h_{c,1}$, but through a tangent bifurcation ($\partial_x F_2(h, x^*) = +1$, in contrast with $\partial_x F_1(h, x^*) = -1$).
- The third-order scheme ($q = 3$) destabilises through a pitchfork bifurcation but at a larger value $h_{c,3} > h_{c,1}$.
- It can be shown that the successive critical values $(h_{c,q})_q$ for schemes of increasing order form an increasing sequence, up to ∞.

Moreover, it can be shown that the implicit scheme embeds all the higher-order schemes of arbitrary orders and can be viewed as an 'infinite-order' scheme (Mendes and Letellier 2004), with no limitation on the time-step size. The price to pay is the implicit nature of the scheme, which means that it is not easily tractable numerically.

3. Lotka–Volterra predator–prey model

Section 2 cast some light on the specificity of discrete dynamics, which cannot be understood in general, even qualitatively, from the behaviour of its continuous counterpart. The same problem also arises in two or more dimensions: the discrete recursion relation following from the continuous evolution law is not unique. The caveats illustrated in Section 2 are all the more relevant.

3.1. *Continuous Lotka–Volterra predator–prey model*

The Lotka–Volterra model is a seminal model in population dynamics and ecology. It was introduced by Lotka in 1920 and independently by Volterra in 1925 to describe the joint evolution of two interacting species, namely preys (population x) and predators (population y) feeding on them (Lotka 1920; Volterra 1931):

$$\begin{cases} \dfrac{dx}{dt} = x(a - by) \\ \dfrac{dy}{dt} = y(cx - d) \end{cases} \tag{15}$$

where a is the growth rate of the prey population alone, by is the mortality rate due to predators (it is taken to be proportional to the predator population y as the natural death of preys is assumed to be negligible), cx is the growth rate of predators (this is determined by predation, and hence proportional to the available resources x), and d is the natural mortality rate of predators. More refined and realistic models have been introduced since, for instance by Kolmogorov and May for ecological studies (Kolmogorov 1936; May 1973). However, for simplicity, we will stick to the basic model since our aim is just to illustrate some caveats with respect to discrete *vs.* continuous modelling.

This model is the archetypical example of nonlinear dynamics inducing intrinsic oscillations. Let us briefly recall its main properties. We will use reduced population and time variables

$$u = \frac{cx}{d}, \qquad v = \frac{by}{a}, \qquad \tau = at \tag{16}$$

so that the coupled evolution becomes

$$\begin{cases} \dfrac{du}{d\tau} = u(1 - v) \\ \dfrac{dv}{d\tau} = \alpha v(u - 1) \end{cases} \tag{17}$$

depending on a single control parameter

$$\alpha = \frac{d}{a}. \tag{18}$$

It possesses two fixed points: an unstable one $(0, 0)$ (a hyperbolic point with unstable direction Ou and stable direction Ov); and a marginally stable one $(u^* = 1, v^* = 1)$. It is well known (Murray 2002) that this 2-dimensional dynamical system leaves the quantity

$$H(u, v) = \alpha u + v - \log(u^\alpha v) = \alpha[u - \log u] + [v - \log v] \tag{19}$$

invariant. Trajectories are thus level curves of $H(u, v)$. A straightforward expansion of $H(u, v)$ around the fixed-point $(u^* = 1, v^* = 1)$ shows that the trajectories in its neighbourhood are close to ellipses with period close to $2\pi/\sqrt{\alpha}$. Further away from (u^*, v^*), the trajectories are still closed (and hence bounded) curves (see the full line in Figure 4) turning in a counterclockwise direction around (u^*, v^*), with extremal amplitudes for u reached when $v = v^* = 1$ (when $u = u^* = 1$, respectively, for v). They describe out-of-phase oscillations of the two species. The period, the phase difference and amplitudes are joint functions of the initial conditions and the control parameter α of the dynamics.

3.2. *Discretisations of the equations*

A natural way to discretise Equation (17) is to use the Euler scheme.

The Euler method

The Euler method, for any given time step h, is given by

$$\begin{cases} u(\tau+h) = u(\tau) + hu(\tau)\,(1-v(\tau)) \\ v(\tau+h) = v(\tau) + h\alpha v(\tau)\,(u(\tau)-1)\,. \end{cases} \tag{20}$$

As an illustration, here is a, very simple, Fortran program corresponding to (20):

```
!  Resolution  of  Lotka-Volterra equations
        implicit none
        real*8 al,h,u,v,u0,v0
        integer i
        al=0.5d0         ! value of alpha
        h=0.1d0          ! time step
        u0=0.3d0          ! initial conditions
        v0=1.d0
        do i=1,250
           u=u0*(1.d0+h*(1.d0-v0))
           v=v0*(1.d0+al*h*(u0-1.d0))
           write(23,*) h*real(i),u,v  ! writing t,u(t),v(t)
           u0=u
           v0=v
        enddo
        end
```

This simply does not work: Figure 4 shows (dotted line) the destabilisation of the expected periodic solution, while Figure 5 displays the growth of the 'constant' $H(u,v)$. We will explain what happens in the analytically tractable case of small amplitude variations in the neighbourhood of the fixed point (u^*, v^*).

Small amplitude

In the harmonic approximation, it is easy to show that

$$H(t+h) = H(t)(1+\alpha h^2) - \alpha h^2(1+\alpha).$$

Then, by recursion,

$$H(nh) = (1+\alpha h^2)^n[H(0) - H_m] + H_m,$$

where $H_m = 1+\alpha$ is the smallest possible value of H. Replacing $(1+\alpha h^2)^n$ by $e^{n\alpha h^2}$ and nh by τ, we get

$$H(\tau) - H_m = e^{\alpha h\tau}\,(H(0) - H_m). \tag{21}$$

This exponential growth of H is shown in Figure 6.

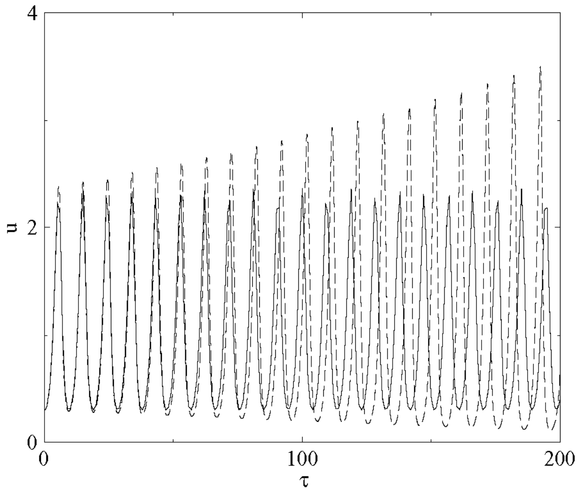

Fig. 4. Trajectories in the phase space $\{\tau, u\}$ for $\alpha = 0.5$. The dotted line corresponds to the Euler scheme, and the full line to the implicit Euler scheme.

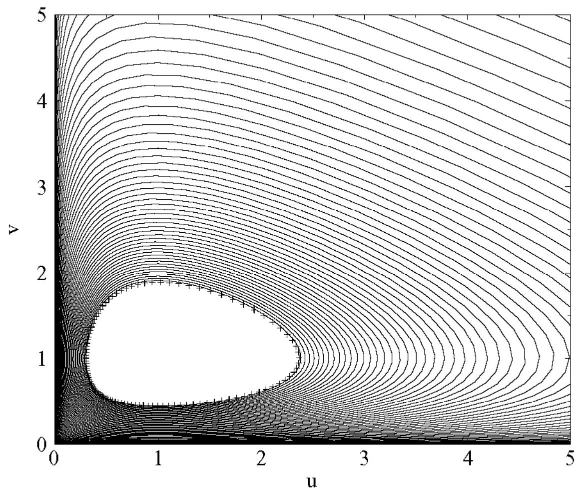

Fig. 5. Trajectories in the phase space $\{u, v\}$ for $\alpha = 0.5$. The continuous line corresponds to the Euler scheme, and the crosses to the implicit Euler scheme.

It is known that the implicit Euler method is often more accurate (Hubbard and West 1991). This leads us to introduce the following hybrid scheme, which differs from Equations (20) in the second line.

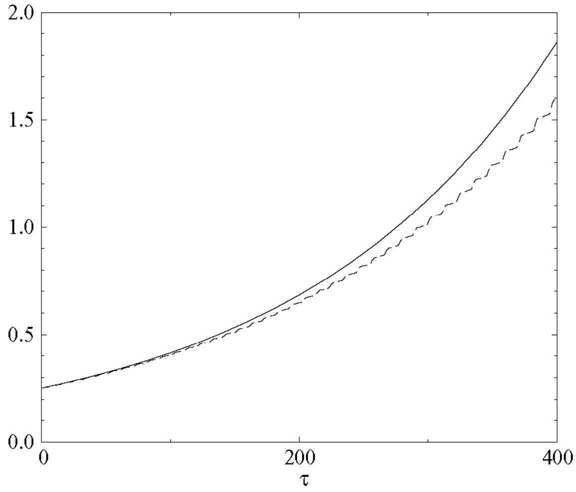

Fig. 6. Exponential divergence of $H(\tau) - H_m$ as a function of $\tau = nh$ with $\alpha = 0.5$, $h = 10^{-2}$. The continuous line is given by Equation (21), and the dashed line shows the results from numerical integration (with $u_0 = 0.3$ and $v_0 = 1$).

The implicit Euler method

$$\begin{cases} u(\tau + h) = u(\tau) + hu(\tau)\,[1 - v(\tau)] \\ v(\tau + h) = v(\tau) + h\alpha v(\tau)\,[u(\tau + h) - 1]\,. \end{cases} \tag{22}$$

This has a simpler Fortran program:

```
do i=1,250
         u=u*(1.d0+h*(1.d0-v))
         v=v*(1.d0+al*h*(u-1.d0))
         write(23,*) h*real(i),u,v  ! writing  t,u(t),v(t)
enddo
```

The results are also displayed in Figures 4 and 5 for comparison. The solution is periodic and h remains bounded, and does not even vary significantly. The implicit Euler scheme is in this case not simply more accurate, but it makes the numerical integration possible (see Figure 7).

3.3. *Symplectic structure*

It is interesting to note that a mere change of variables allows us to unravel the *Hamiltonian character of the Lotka–Volterra equations*, that is, the underlying symplectic structure of this conservative dynamics. Indeed, setting

$$p = \log u \quad \text{and} \quad q = \log v \qquad \text{(hence } H = \alpha(e^p - p) + (e^q - q)) \tag{23}$$

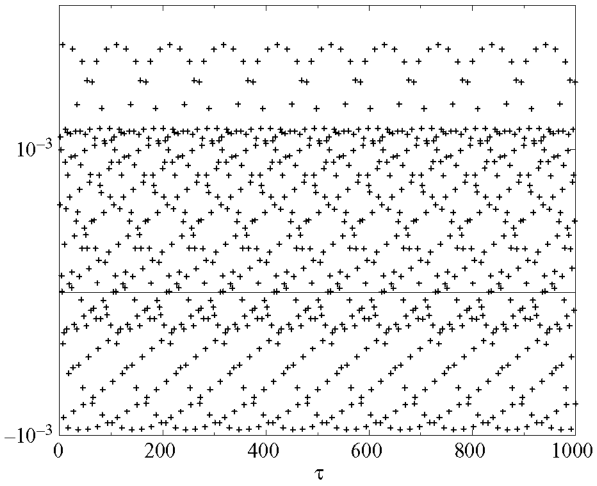

Fig. 7. Stability of $H(\tau) - H(0)$ as function of $\tau = nh$ with $\alpha = 0.5$. Numerical integration of Equations (22). Notice the scales.

casts the evolution (17) into the Hamilton equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q}. \tag{24}$$

The reason underlying the need to use the implicit Euler scheme to solve the discrete Lotka–Volterra equation properly is thus known: it is the symplectic structure of the equation given by the Hamilton equations (see, for instance, Tabor (1989)):

$$\begin{cases} \dot{p} = -\dfrac{\partial H}{\partial q} \\ \dot{q} = \dfrac{\partial H}{\partial p}. \end{cases} \tag{25}$$

The Euler scheme (with the same notation as above: $p_n \equiv p(t_n)$ and $q_n \equiv q(t_n)$ where $t_n = t_0 + nh$) is given by

$$\begin{cases} p_{n+1} = p_n - h\dfrac{\partial H}{\partial q}(p_n, q_n) \\ q_{n+1} = q_n + h\dfrac{\partial H}{\partial q}(p_n, q_n). \end{cases} \tag{26}$$

The Jacobian of the associated linear transformation is

$$J = 1 + h^2 \left[\frac{\partial^2 H}{\partial q^2}\frac{\partial^2 H}{\partial p^2} - \left(\frac{\partial^2 H}{\partial q \partial p} \right)^2 \right].$$

This means that the phase-space volume is not conserved in time (unlike the case for the continuous evolution, where it is conserved). In the most frequent case, for which the variables p and q in the Hamiltonian can be separated, namely $H(p, q) = K(p) + V(q)$, the implicit Euler method

$$\begin{cases} p_{n+1} = p_n - \dfrac{\partial H}{\partial q}(p_n, q_n) \\ q_{n+1} = q_n + \dfrac{\partial H}{\partial p}(p_{n+1}, q_n) \end{cases} \tag{27}$$

fixes this flaw. Namely, plugging $p_{n+1} = p_n - h(\partial H/\partial q)(p_n, q_n)$ into the expression for q_{n+1} before taking the derivative leads to $J = 1$. Such an integration scheme is called a *symplectic integrator*, or the *symplectic Euler method*, since it preserves the symplectic structure of the original evolution, and the associated area conservation (Sanz-Serna 1992). Note that the symplectic structure is only apparent in the canonical variables $p = \log u$, $q = \log v$.

4. A historical precedent: Newton's derivation of Kepler's laws

The above situation for the Lotka–Volterra model resembles Newton's resolution of the planetary movement equation. The physical requirement to use a semi-implicit scheme is again encountered in the reasoning developed by Newton to provide dynamical grounds for Kepler's laws (Coullet *et al.* 2004).

In his *Principia*, in 1687, Isaac Newton implemented a discrete description of the planetary motion as the result of a sequence of pointwise impulses, which he actually borrowed from Robert Hooke. Remarkably, the algorithm implicitly associated with this viewpoint corresponds to an implicit version of the Euler discretisation scheme in the plane (Coullet *et al.* 2004)

$$\begin{cases} \vec{r}_{n+1} = \vec{r}_n + h\vec{v}_n \\ \vec{v}_{n+1} = \vec{v}_n + h\,\dfrac{\vec{f}(r_{n+1})}{m} \end{cases} \tag{28}$$

(where m is the planet mass and f the central gravitation force) and it achieves a better numerical stability than the standard one. Indeed, the standard Euler algorithm

$$\begin{cases} \vec{r}_{n+1} = \vec{r}_n + h\vec{v}_n \\ \vec{v}_{n+1} = \vec{v}_n + h\,\dfrac{\vec{f}(r_n)}{m} \end{cases} \tag{29}$$

fails to follow the planetary motion properly, mainly because it fails to preserve conservation laws (energy conservation and the equality of areas swept in a given time interval). It is worth noting that the celebrated Verlet algorithm used in molecular dynamics simulations follows (28) and not the Euler scheme (29).

5. Discusssion and extensions

5.1. *Improved discretisation schemes*

We have briefly mentioned the improved validity range of Euler implicit schemes (see Section 2.5). In the same spirit, a wide variety of generalised discretisation procedures, known as *non-standard Euler schemes*, are still in development, but mainly on the basis of numerical skill and intuition. A few empirical guidelines can be summarised (Mickens 2002):

— The discrete scheme should be of the same (differential) order as the original continuous evolution equation.
— The invariants and symmetries of the continuous evolution should be preserved. This is the basic principle of so-called *geometric integrators*. Two examples have been given here: the symplectic integrators associated with the Lotka–Volterra equations and Newton equations, respectively (Hairer *et al.* 2002);
— Nonlinear terms (for example, quadratic cross-products) are better treated using a hybrid expression. For instance, a term $x(t)y(t)$ in dy/dt might be best translated into a term $x_{n+1}y_n$ (rather than $x_n y_n$) in the expression for $y_{n+1} - y_n$.
— Generally speaking, the discretisation step h should never exceed the characteristic times of the continuous evolution.

5.2. *Conclusion*

We began this paper by presenting an example showing explicitly the link between the validity of the discretisation scheme and the dynamical (in)stability of the associated map for a unit step-size. Conversely, our study has cast light on the specificity of the discrete dynamics, which, in general, cannot be understood, even qualitatively, from the behaviour of its continuous counterpart. In dimension $d \geqslant 2$, the discretisation of a system of first-order differential equations is not unambiguously defined. In the cases of the Lotka–Volterra (predator–prey) model and Newton's equations, we showed how the symplectic structure of the equation determines the 'good' choice. More generally, these examples illustrate the deep difference between continuous dynamical systems and discrete recursions, and, accordingly, the gap existing between a continuous dynamical system and its numerical integration, which requires a discrete scheme that might not be a faithful analogue from either a conceptual viewpoint or even for simple practical purposes.

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