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

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Abstract

The relation between continuous-time dynamics and corresponding discrete schemes, and its generally limited validity, is an important and widely acknowledged chapter of numerical analysis. In this paper, we propose another, more physical, viewpoint on this topic in order to understand the possible failure of discretization procedures and the way to fix it. Three basic examples, the logistic equation, the Lotka-Volterra predator-prey model and the Newton 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 *MSCS* is devoted to the ubiquitous duality between discreteness and continuity, and to the debates arising either to reconcile, or to contrast, these two notions. We shall consider this issue within a more restricted scope: in all this paper, "continuous" and "discrete" will refer to *time*, and to the modality used to describe a *deterministic* evolution: either by a continuous trajectory $t \in [0, \infty[\rightarrow x(t)$, either as a discrete sequence $(x_n)_n$ labeled with integers. Our aim is mainly to give a simple and comprehensive account of results scattered in the literature.

A striking difference between discrete and continuous modelings, explained in Sec. 2, is related to the *occurrence of deterministic chaos*, namely of a seemingly erratic behavior originating in nonlinear amplification of any perturbation (sensitivity to initial conditions) and mixing of phase space regions. Discrete autonomous dynamical systems in 1-dimension can exhibit chaotic behavior, whereas the corresponding (1-dimensional) continuous evolution equations rule it out, and cannot even possess a nontrivial periodic solution. A phase-space dimension $d \geq 3$, at least, is required to (possibly) observe a chaotic behavior in a continuous dynamical system (see for instance the textbook [Devaney 1989]). This point hints at the following issue: the passage from discrete to continuous equations, or conversely, is all but insignificant. Moreover, this issue should unavoidably be faced, since any numerical resolution of a continuous equation in fact *imply the recourse to a discrete analog*: it is thus of the utmost importance to describe the relation between the desired (continuous) solution and the output of the actual (discrete) computation.

In Section 2, we evidence some caveats about 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 modelings, providing a physical interpretation of standard numerical analysis procedures. In Section 3, we consider a 2-dimensional evolution, which brings new difficulties. Some guidelines might be drawn 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. A final Section 5 draws 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 that a, the Malthus coefficient characterizing the growth of the population

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

has to decrease when X_n increases, due to resources limitation [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 through the change of variable $x_n = X_n/M$. A very rich variety of dynamic behaviors is generated by this Equation (1), whose temporal structure is governed by the values of the control parameter a. Since the seminal reference[1] [May 1976], several studies of the asymptotic dynamics of (1) have been published, among which some very pedagogical ones are [Evans and Morriss 1991], [Peitgen et al. 1992], [Korsch and Jodl 1998]. Let us only recall the most significant properties.

For a given, such that $1 < a < a_1 = 3$, the fixed point $x_a^* = 1 - 1/a$ is stable, globally attractive, therefore $x_n \to x_a^*$ as $n \to \infty$, irrespectively of the initial condition x_0 provided it belongs to its basin of attraction $]0, 1[$. In $a_1 = 3$, a cycle of period 2 appears through a pitchfork bifurcation. Also called period-doubling bifurcation since it is associated with the destabilization of a fixed point x_a^* into a 2-cycle (or the destabilization of a 2^n-cycle into a 2^{n+1}-cycle when it involves $f_a^{2^n}$ instead of f_a), this generic bifurcation is characterized by the relation $f'_{a_1}(x^*_{a_1}) \equiv \partial_x f(a_1, x^*_{a_1}) = -1$ and the generic condition $\partial^2_{ax} f(a_1, x^*_{a_1}) \neq 0$ (denoting here the a-dependence on the same footing for the sake of clarity) [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 destabilizes 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 (1) is actually a generic example exhibiting this so-called period-doubling scenario toward chaos, i.e. a normal form to which any one-parameter family experiencing such a scenario is conjugated [Collet and Eckmann 1981]. In $a = a_\infty$, a chaotic behavior arises, reflecting 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 (but now understood [Collet and Eckmann 1981]) with non chaotic regions where stable odd cycles rule the asymptotic dynamics.

The conclusion is now acknowledged, but it was striking at the time

[1] Without lowering the historical importance and repercussions of this paper, it is to note that more is known today on the asymptotic behavior in the region $a > a_\infty$, which leads to modify May's claim that all trajectories are periodic but with period so large that the dynamics resembles chaos.

of publication of [May 1976]: a large variety of chaotic behaviors 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 with 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 carry on the analysis in this direction.

2.2 Continuous-time counterpart: a trivial dynamics

As it is impossible to give an analytical solution[2] of (1), i.e. 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 to 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 analytical solution is easily obtained :

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

This solution is obviously regular with respect to $t \geq 0$ for any value of $a > 1$ and, not surprisingly, tends to x_a^* as $t \to \infty$. In contrast with this plain behavior, qualitatively insensitive to the value of $a > 1$, any attempt to solve (2) by discretization 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). How is it possible ? We have therefore to quantify what means "*small enough*".

[2] Except for $a = 4$, 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 to prove that one gets a fully chaotic behavior 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).

2.3 Interpretation of discretization schemes associated with the logistic equation

Let us thus recall the behavior of the discretization schemes associated with (2) [Borrelli and Coleman 1998]. Our aim is evidently not to get more knowledge about this equation, nor to device an accurate numerical resolution, but rather to understand in this tractable and well-understood situation what is currently done to solve real problems when no straightforward solution is available. For a given time step h, the discretization scheme writes

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

A remarkable feature of the logistic equation is the possibility to rewrite 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 for evolution (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 a whole period-doubling scenario when the discretization step h increases, namely at values $(h_k)_k$ with $A(a, h_k) = a_k$, i.e.

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

Chaos arises 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 ($a_k =$

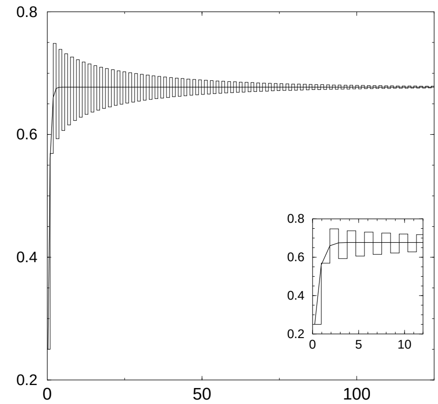

Figure 1: Discretization of the logistic equation (2) with $a = 3.1$, using a time step $h < h_c$ (here $h = 0.94$ whereas $h_c \equiv 2/(a-1) = 20/21 \approx 0.95$), see text, Section 3. Bold line: exact (continuous-time) solution of (2). Stair step $\frac{1}{\lambda} f_A(nh)$. $x_a^* = 1 - 1/a$. Behavior near origin is shown in the inset.

$1+(a-1)h_k$). In particular, it is interesting to note that the sequence $(h_k)_k$ follows the same universal scaling law $h_\infty - h_k \sim \delta^{-k}$ or more precisely:

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

For illustration let us 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 the 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 behavior can be suppressed by replacing a discrete model by its limiting continuous counterpart, or conversely destabilization of the continuous-time evolution, leading to cycles and even a spurious chaotic behavior, might follow from an improper choice of the step of the discretization [Yamaguti and Matano 1979].

Nevertheless, 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

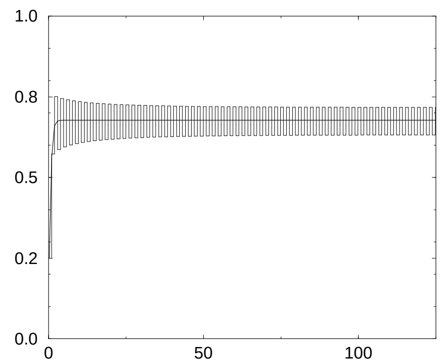

Figure 2: Same as Fig. 1 but with $h = 0.96 > h_c$.

our discussion, we shall now investigate what remains true in 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^* (i.e. $f(x^*) = x^*$ and $|f'(x^*)| < 1$). The naive continuous counterpart writes $dy/dt = f(y) - y$. Linear stability analysis shows that x^* is still a (at least locally) 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 discretization scheme destabilizes 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 $h = h_c$ (the additional generic condition for this bifurcation stated in Sec. 2.1 is also fulfilled, as can be directly checked).

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 instable 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 $dy/dt = f_a(y) - y$ to capture the behavior of the discrete one $x_{n+1} = f_a(x_n)$. It is to note that, in the case when $f'_a(x^*_a)$ decreases with a (as in

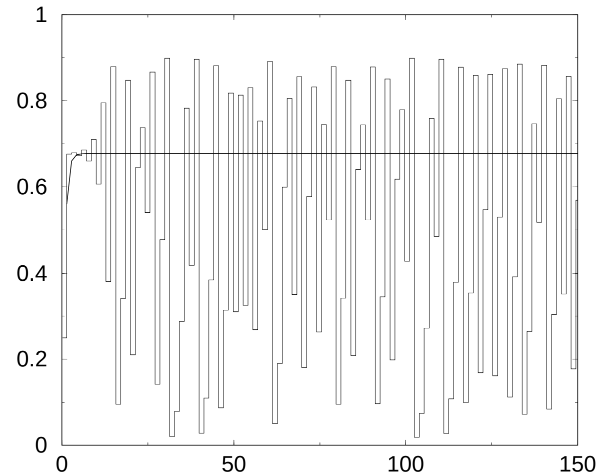

Figure 3: Discretization of the logistic equation (2) with $a = 3.1$, using a time step $h = 3/(a-1) = 1.424$ corresponding to the fully chaotic case $A = 4$, see text, Sec. 2.3.

the logistic example), then $h_c(a)$ decreases if a increases: the more stable is the fixed point (i.e. the larger $|f'_a(x^*_a) - 1|$ with $f'_a(x^*_a) - 1 < 0$), the smaller is the time-step range of validity of the discretization scheme (in a sense, the less stable is the discretization scheme).

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

The explanation lies in the comparison of the intrinsic time scale(s) of the dynamics with the chosen "time unit" h. The characteristic time of a continuous evolution, still denoted $dy/dt = f(y) - y$ to avoid proliferation of new notations, can be estimated as $\tau \sim 1/[1 - f'(x^*)]$. Indeed, a mere linearization 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 $x(t) - x^* \sim e^{-t[1-f'(x^*)]}$ hence the value of τ. Destabilization of the discretization scheme occurs when $h > h_c = 2\tau$. The stepwise updating, after each time step h, of the evolution law is too rough to properly control the discrete evolution and 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 properly sample the continuous trajectory.

It is to 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, f and $\phi^{-1} \circ f \circ \phi$ (providing an equivalent modeling of the discrete model associated with f) have the same critical value h_c and the same characteristic time τ. Indeed, denoting $y^* = \phi^{-1}(x^*)$ the fixed point of $\phi^{-1} \circ f \circ \phi$, it is straightforward to check that $f'(x^*) = [\phi^{-1} \circ f \circ \phi]'(y^*)$, from which follows the equality of the characteristic time associated respectively to f and $\phi^{-1} \circ f \circ \phi$.

Let us carry further the comparison between the continuous evolution and its discretization, 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, let us consider an heating/cooling device, able to measure the difference between the instantaneous room temperature and a prescribed one, and to monitor the appropriate energy supply or extraction, to compensate the measured difference. If the time h necessary for the device to actually deliver the required energy is longer that 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 superimpose 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 Sec. 2.3 is the mathematical translation of this ubiquitous phenomenon.

2.5 Generalized Euler discretization schemes

Actually, the improvement of the validity range of a discretization scheme by using an implicit recursion relation is a general property. In particular, implicit scheme (with the notation $x_n \equiv x(t_n)$ where $t_n = t_0 + nh$)

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

for the logistic equation can be checked to be stable for arbitrarily large time steps h [Hubbard and West 1991].

Let us illustrate the general ideas on the simpler case of a 1-dimensional dynamical system $dx/dt = g(x)$ having a stable fixed point x^*, i.e. $g(x^*) = 0$ and $g'(x^*) < 0$. The first order Euler scheme $z_{n+1} = z_n + hg(z_n)$ destabilizes in $h_c = 2/|g'(x^*)|$ through a pitchfork bifurcation (see Sec. 2). Higher-order schemes write

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

Direct computation of $\partial_x F_q(h, x^*)$ yields the following results
— the second-order scheme ($q = 2$) destabilizes in the same value $h_{c,2} = h_{c,1}$ but now 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 ($q = 3$) destabilizes through a pitchfork bifurcation but at a larger value $h_{c,3} > h_{c,1}$;
— it can be checked 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 implicit scheme embeds all the higher-order schemes of arbitrary orders and can be seen 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, not easily tractable numerically.

3 Lotka-Volterra predator-prey model

The previous Section 2 has enlightened the specificity of discrete dynamics, that cannot in general be understood, even qualitatively, from the behaviour of its continuous counterpart. In two or more dimensions, the same problem arises: 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

Lotka-Volterra model is a seminal model in population dynamics and ecology, 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]:

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

a is the growth rate of the prey population alone, by is the mortality rate due to predators hence proportional to the predator population y (natural death of preys is supposed to be negligible); cx is the growth rate of predators, allowed by predation, 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]. We here stick to this basic model for the sake of its simplicity, having the aim to illustrate some caveats in discrete *vs* continuous modeling.

This model is the archetype of nonlinear dynamics inducing intrinsic oscillations. Let us briefly recall its main properties. Using reduced population and time variables

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

so that the coupled evolution writes

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

depending on a single control parameter

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

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

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

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 neighborhood are close to ellipses, and of period close to $2\pi/\sqrt{\alpha}$. Farther from (u^*, v^*), trajectories are still closed (hence bounded) curves (see Figure 4 full line) turning around (u^*, v^*) counterclockwise, with extremal amplitudes for u reached when $v = v^* = 1$ (respectively when $u = u^* = 1$ 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 Discretizations of the equations

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

<u>Euler method.</u> It writes, for any given time step h

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

We give for illustration the - very simple - corresponding Fortran program.

```
!  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
```

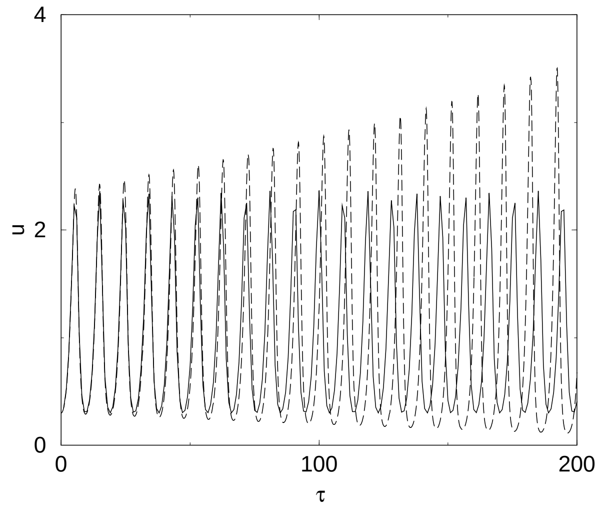

Figure 4: Trajectories in the phase space $\{\tau, u\}$ for $\alpha = 0.5$. Dotted line corresponds to the Euler scheme, full line to the implicit Euler scheme.

```
    v0=v
enddo
end
```

It simply does not work: Figure 4 shows (dotted line) the destabilization of the expected periodic solution whereas Figure 5 displays the growing of the "constant" $H(u, v)$. Let us explain what happens in the analytically tractable case of small amplitude variations in the neighborhood 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 one gets

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

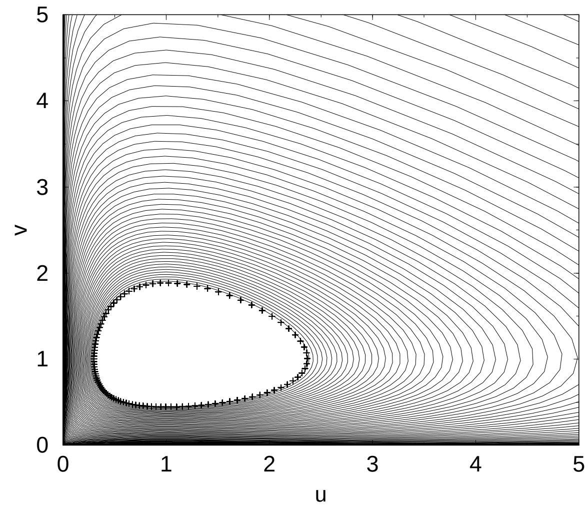

Figure 5: Trajectories in the phase space $\{u, v\}$ for $\alpha = 0.5$. Continuous line corresponds to the Euler scheme, crosses to the implicit Euler scheme.

This exponential growing of H is shown in Figure 6.

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

Implicit Euler method

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

with 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. Implicit Euler scheme is in this case not simply more accurate, but it makes the numerical integration possible (see the Figure 7).

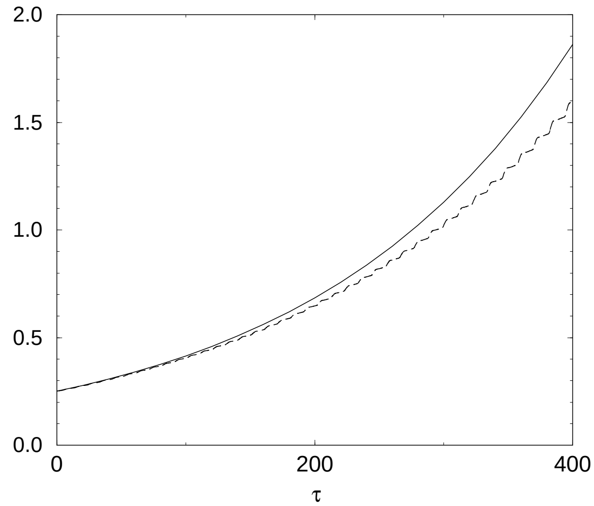

Figure 6: *Exponential divergence of* $H(\tau) - H_m$ *as function of* $\tau = nh$. $\alpha = 0.5$, $h = 10^{-2}$. *Continuous line is given by Equation (21), long dotted line results from numerical integration (with* $u_0 = 0.3$ *and* $v_0 = 1$*).*

3.3 Symplectic structure

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

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

casts the evolution (17) into Hamilton equations:

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

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

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

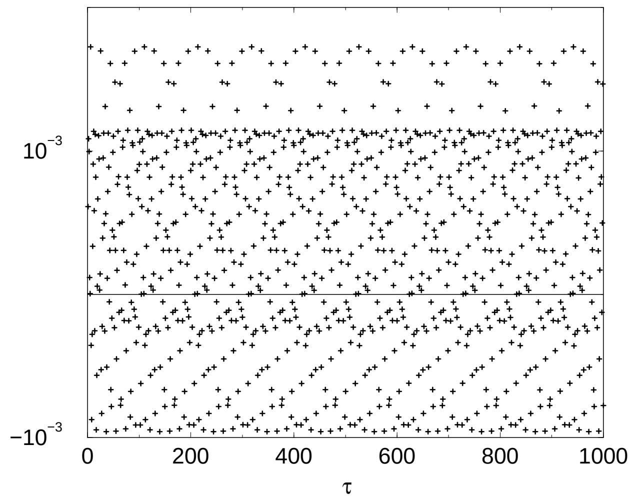

Figure 7: Stability of $H(\tau) - H(0)$ as function of $\tau = nh$ with $\alpha = 0.5$. Numerical integration of Equations (22). Notice the scales.

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

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

The Jacobian of the associate linear transformation is

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

It means that the phase-space volume is not conserved in time (in contrast to its conservation in the continuous evolution). In the most frequent case when there is separation of the variables p and q in the Hamiltonian, namely $H(p, q) = K(p) + V(q)$, the implicit Euler method

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

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

4 An historical precedent: Newton derivation of Kepler laws

The above situation of Lotka-Volterra model resembles the resolution of the planetary movement equation as done by Newton. The physical requirement to use a semi-implicit scheme is yet encountered in the reasoning developed by Newton to provide dynamical grounds to Kepler laws [Coullet et al. 2004].

In its *Principia*, in 1687, Isaac Newton implemented a discrete description of the planetary motion as resulting of a sequence of pointwise impulses, that he actually borrowed from Robert Hooke. Remarkably, the algorithm implicitly associated with this viewpoint corresponds to an implicit version of Euler discretization 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 properly the planetary motion, mainly because it fails to preserve conservation laws (energy conservation and equality of areas swept in a given time interval). It is remarkable 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 discretization schemes

We have briefly mentioned the improved validity range of Euler implicit schemes (see Sec. 2.5). In the same spirit, a large variety of generalized discretization procedures, known as *non standard Euler schemes*, are still in development, mainly on the basis of numerical skill and intuition; a few empirical guidelines can be summarized [Mickens 2002]:

— the discrete scheme should be of the same (differential) order than the original continuous evolution equation;

— invariants and symmetries of the continuous evolution should be preserved: this is the basic principle of the so-called *geometric integrators*; two examples have been given here with the symplectic integrators associated respectively with Lotka-Volterra equations and Newton equations [Hairer et al. 2002];

— nonlinear terms (e.g. quadratic cross-products) are better treated using an 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_ny_n) in the expression for $y_{n+1}-y_n$;

— mainly, the discretization step h should never exceed the characteristic times of the continuous evolution.

5.2 Conclusion

We have presented first an example showing explicitly the link between the validity of the discretization scheme with the dynamical (in)stability of the associated map for a unit step-size. Convertely, our study enlightens the specificity of the discrete dynamics, that cannot in general be understood, even qualitatively, from the behaviour of its continuous counterpart. In dimension $d \geq 2$, discretization of a system of first-order differential equations is not unambiguously defined. In the cases of Lotka-Volterra (predator-prey) model and Newton 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, following in fact a discrete scheme that might not be a faithful analog, not only from a conceptual viewpoint, but even for plain practical purposes.

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