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Note

A Horror Story about Integration Methods

INTRODUCTION

Difference schemes for numerical integration can look simple and robust, yet have insidious features that bring their real utility into question. Two simple schemes are explored here, and each is applied to the problem of the physical pendulum. One of the methods is symplectic, while the other gives rise to an attracting set, something forbidden for a bounded Hamiltonian system like the pendulum. The contrast provides a vivid example, useful for didactic purposes, that illustrates the need for care in matching integration methods to problems.

The first of the two systems is the time-centered leapfrog:

$$\begin{aligned} u^{(n+1/2)} &= u^{(n-1/2)} + Tf^{(n)}, \\ x^{(n+1)} &= x^{(n)} + Tu^{(n+1/2)}, \end{aligned} \tag{1}$$

and the second is a simple predictor-corrector:

$$\begin{aligned} x_p &= x_n + Tu_n, \\ u_{n+1} &= u_n + \frac{T}{2}(f(x_n) + f(x_p)), \\ x_{n+1} &= x_n + \frac{T}{2}(u_n + u_{n+1}) = x_p + \frac{T^2}{4}(f(x_n) + f(x_p)). \end{aligned} \tag{2}$$

Momenta per unit mass (velocities in cartesian coordinates) are denoted by u, coordinates by x, forces per unit mass (accelerations) by f, and T is used for the integration timestep. Values at the old timestep are denoted by n, those at the new by $n+1$, and at the predicted position by p. The use of superscripts in one situation and subscripts in the other conforms to standard usage in gravitational problems. The leading error term is $O(T^3)$ with either method. The time-centered leapfrog has been widely used in both plasma and gravitational n-body problems, and the predictor-corrector has been used for some gravitational problems. The leapfrog was introduced into gravitational problems [1, 2] as a means of coping with the chaotic property of those problems [3, 4] because it is reversible and it has an exact Liouville theorem. Both schemes generalize to three dimensions by regarding x, u, and f as vectors.

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Are These Methods Symplectic?

An integration method is said to be symplectic if the state of the system following an integration step could have been reached from that before the step by some canonical transformation. This is important because Hamiltonian systems are not structurally stable in the mathematical sense: an arbitrary displacement in the phase space need not be consistent with the Hamiltonian equations.

The most succinct way to test whether a method is symplectic is to verify the Poisson-bracket relations between the before and after states. Those relations may conveniently be written in matrix form as follows [5, 6]. Let the Jacobian matrix that leads from "before" to "after" be

$$M = \frac{\partial(x^{(n+1)}, u^{(n+1/2)})}{\partial(x^{(n)}, u^{(n-1/2)})}.$$

In an s-degrees of freedom problem, M is of dimension $2s \times 2s$; it is simply 2×2 for present purposes. Introduce now the matrix constructed of four blocks,

$$J = \begin{pmatrix} O_s & I_s \\ -I_s & O_s \end{pmatrix},$$

where I_s is the $s \times s$ identity and O_s is an $s \times s$ matrix all of whose elements are zero. The matrix M is symplectic (as is the transformation it represents) if

$$M^{\mathrm{T}} J M = J, \tag{3}$$

and the corresponding transformation is canonical. The superscript T denotes matrix transpose.

A bit of writing can be saved for the present case ($s = 1$, 2×2 matrices) with the notation

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix};$$

then $M^{\mathrm{T}} J M = J(AD - BC)$, so the transformation is symplectic if $\det |M| = 1$. (Warning: this works *only* for $s = 1$, 2×2 matrices!) Also denote df/dx evaluated at the point $x^{(n)}$ by $f'(x^{(n)})$.

The leapfrog gives

$$A = \frac{\partial x^{(n+1)}}{\partial x^{(n)}} = 1 + T^2 f'(x^{(n)}),$$

$$B = \frac{\partial x^{(n+1)}}{\partial u^{(n-1/2)}} = T,$$

$$C = \frac{\partial u^{(n+1/2)}}{\partial x^{(n)}} = T f'(x^{(n)}),$$

$$D = \frac{\partial u^{(n+1/2)}}{\partial u^{(n-1/2)}} = 1,$$

from which it is clear that the method is symplectic for any differentiable $f^{(n)}$. The fact that momenta and coordinates are associated with different physical times is not important for this formal manipulation. The leapfrog is also symplectic in three dimensions.

The predictor-corrector, Eq. (2), is a little more complicated. Forces are evaluated at two different places (and times): at x_n and at $x_p = x_n + u_n T$. Introduce the notations, $F = f'(x_n)$, $G = f'(x_n + u_n T)$, and let $\tau = T/2$. Then

$$A = \frac{\partial x_{n+1}}{\partial x_n} = 1 + \tau^2(F + G),$$

$$B = \frac{\partial x_{n+1}}{\partial u_n} = 2\tau(1 + \tau^2 G),$$

$$C = \frac{\partial u_{n+1}}{\partial x_n} = \tau(F + G),$$

$$D = \frac{\partial u_{n+1}}{\partial u_n} = 1 + 2\tau^2 G$$

which, after a little algebra, gives

$$AD - BC = 1 + \tau^2(G - F).$$

This requires either $\tau = 0$ (undesirable because it means zero timestep) or $G = F$ (or both) in order to have $AD - BC = 1$, as required for a symplectic method. The condition, $G = F$, says $f'(x_n) = f'(x_n + u_n T)$, or that the derivative of force by position at the two different places (and times) must be the same. That condition requires something no more complicated than a harmonic oscillator force law, $f = -kx$; the predictor-corrector is not symplectic for more general force laws.

Both the predictor-corrector and the leapfrog integrate the harmonic oscillator exactly in the sense that $x^{(n)} = X\cos(n\Omega T)$, inserted into either scheme, along with $f = -kx$ satisfies the scheme exactly with

$$T^2 k = 4\sin^2(\Omega T/2).$$

The integration becomes unstable for $T^2 k > 4$. A second independent solution, with the same stability limit, is obtained with the substitution $x^{(n)} = X\sin(n\Omega T)$.

A problem somewhat more complicated than the harmonic oscillator is needed to explore differences between the two methods. The physical pendulum provides such an example.

The Physical Pendulum

The physical pendulum has two fixed points: that with the pendulum at rest pointing down is stable while that with it at rest pointing up is unstable. The phase plane is well known: the neighborhood of the stable fixed point looks like a harmonic oscillator. Low-energy orbits are confined to this neighborhood. A pair of separatrix trajectories crosses at the unstable fixed point. Orbits with energy greater than that of the separatrix rotate: the pendulum zips past the vertically upright position and continues in the same direction. The phase space lies on a cylinder, periodic in angle and unbounded in angular momentum.

The force for the physical pendulum may be written, $T^2 f = K \sin\theta$ with $K > 0$, so $\theta = 0$ when the pendulum points upward. This strange convention makes the notation conform to the literature. Change the notation a bit more, using I_n for $Tu^{(n-1/2)}$ and so on, and the leapfrog takes the form,

$$\begin{aligned} I_{n+1} &= I_n + K \sin \theta_n, \\ \theta_{n+1} &= \theta_n + I_{n+1}. \end{aligned} \tag{4}$$

This system will be recognized as the standard, or Chirikov, map familiar from chaos theory [7]. The physical pendulum is a useful example because its difference form (the Chirikov map) has been so well studied.

The angle, θ, can be reduced modulo 2π, and the second of Eqs. (4) implies that I can be similarly reduced for most purposes. The phase plane extends over $(0, 2\pi)$ in both θ and I. This map has some strange and well-known properties. Plots are shown in Lichtenberg and Lieberman [7] for several different values of K. Its important features are (1) it is area-preserving (e.g., no attractors), even though orbits may break up and become stochastic, and (2) it has two fixed points that correspond to those of the pendulum: a stable fixed point at $\theta = \pi$, $I = 0$ (pendulum at rest pointing down, stable for $K < 4$) and an unstable fixed point at $\theta = 0$, $I = 0$ (pendulum at rest pointing up). In addition, it has a pair of (stable) period-2 fixed points at $\theta = 0$, $I = \pi$ and at $\theta = \pi$, $I = \pi$. These are of interest to compare to the map that follows from the predictor-corrector. Additional fixed points of higher order can appear at certain amplitudes, those for which the integrator just happens to produce periodic orbits. These are not important for present purposes.

The predictor-corrector difference equations for the physical pendulum become

$$\begin{aligned} \theta_p &= \theta_n + I_n, \\ I_{n+1} &= I_n + \frac{K}{2}(\sin \theta_n + \sin \theta_p), \\ \theta_{n+1} &= \theta_n + \tfrac{1}{2}(I_n + I_{n+1}). \end{aligned} \tag{5}$$

This system was explored computationally. Plots showed a systematic drift toward $I = \pi$, which suggested a closer look at that neighborhood. If $I = \pi$, θ_p becomes $\theta_n + \pi$ (reduced mod 2π) in the first line, so $(\sin\theta_n + \sin\theta_p) = 0$ identically and finally $\theta_{n+1} = \theta_n + \pi = \theta_p$ for any value of θ_n whatsoever. Thus every point on the line, $I = \pi$, is a period-2 fixed point whatever the value of K. There is an infinite number of period-2 fixed points on that line. This is quite different from the

Chirikov map, which has only two fixed points at $I=\pi$. The line of fixed points cuts the phase plane into two parts.

Look at motions near one of these fixed points in first order. Pick some value for $\theta=\alpha$, say, and take $I=\pi$. Describe the departures by $\theta_n=\alpha+\delta$, $I_n=\pi+\varepsilon$. Then $\theta_p=\alpha+\delta+\pi+\varepsilon$, so $\sin\theta_n+\sin\theta_p=-\varepsilon\cos\alpha$ to first order in δ and ε. New values of δ and ε may be obtained by multiplying the original values by the matrix (with the π in the θ term omitted):

$$\begin{pmatrix} 1 & -\frac{K}{4}\cos\alpha \\ 0 & 1-\frac{K}{2}\cos\alpha \end{pmatrix}.$$

Two steps should be used to return to the neighborhood of the starting point. On a second step, the same matrix applies but the $\cos\alpha$ terms change sign because α must be replaced by $\alpha+\pi$. The result of both steps is obtained from the matrix product (+ signs on the left, − signs on the right) to yield

$$\begin{pmatrix} 1 & -\frac{K^2}{8}\cos^2\alpha \\ 0 & 1-\frac{K^2}{4}\cos^2\alpha \end{pmatrix}. \tag{6}$$

This last matrix has one eigenvalue equal to one and the other less than unity. The decreasing direction corresponds to motions toward the line $I=\pi$, indicating that that line is an attracting set. It is not a strange attractor.

Numerical checks suggest that the entire domain is a basin of attraction toward the attracting set. In evaluating numerical integration methods, the number of

FIG. 1. Standard (Chirikov) map iterated 128 times with $K=0.5$.

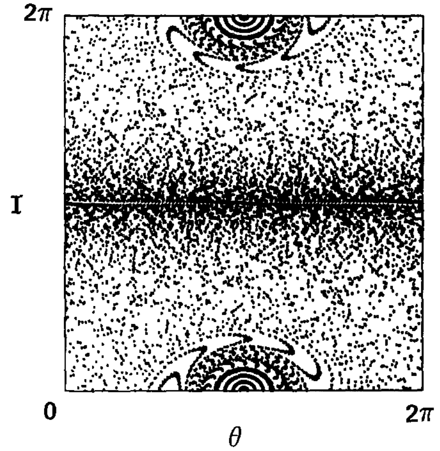

FIG. 2. Predictor-corrector map iterated 128 times with $K = 0.5$ from the same starting condition used for Fig. 1.

integration steps required to reach the attractor is important. It tells how long an integration may be carried on before significant error builds up. Ten or twenty integration steps cause appreciable drift toward the attracting set over much of the (θ, I) plane. Near the two fixed points of the pendulum, at $\theta = \pi$, $I = 0$ and at $\theta = 0$, $I = 0$, the force field is asymptotically harmonic and the integration is much better.

These difference schemes may be iterated over and over. We show in Figs. 1 and 2 a comparison of results obtained in 128 iterations of the Chirikov map (Fig. 1) and of the predictor-corrector (Fig. 2). Both maps started with 64 points equally spaced along a line at $\theta = \pi$ and extending from 0 to 2π in I. The plot shows all 128 images of each of the 64 points. Very little evidence for the integrability of the underlying physical problem remains in Fig. 2, although it is quite apparent in Fig. 1. The empty band near the attracting set in Fig. 2 results from the short run and the starting condition used. It fills in if the map is iterated more times.

Migration toward the attracting set is slower with shorter timesteps. The constant K goes as T^2 for shorter timesteps, and the matrix (6) shows that points near the attracting set move closer by an amount depending on K^2 (proportional to T^4) per integration step. Since more integration steps are needed to reach a given physical time with shorter timesteps, those points move closer by an amount depending on T^3 in a given physical time interval. The attracting set remains, however. It simply takes a bit longer to produce catastrophic results.

COMMENTS

The character of the problem has changed completely in going from the physical problem to the predictor-corrector because there is an attracting set in the phase space represented by the predictor-corrector. Three levels have been investigated. First, the physical problem is Hamiltonian. It cannot have any attracting sets. Next we integrate that by the leapfrog, which is symplectic, and still there are no attracting sets. But an attracting set appears at the third level when it is integrated by the predictor-corrector. An essential part of the physics has been lost. Since both methods are correct through $O(T^2)$, it is clear that higher-order (ignored) terms have conspired to produce the attractor. A symplectic method, with a consequent Liouville theorem, tries to guarantee that that particular phenomenon will not occur.

Symplectic difference methods have been of some interest in recent years [8–10] and faithful rendering of invariant curves is presented as evidence that these methods perform better than their conventional competitors. We see here that difference methods usually perform better near invariant curves than elsewhere and that faithful rendering in regions far from fixed points or invariant curves can provide a more stringent test. Symplectic methods may, in fact, represent more of an improvement than implied from the test results presented. Unfortunately, one rarely knows what the motion should be far from fixed points or invariant curves in examples more complicated than the physical pendulum.

Symplectic methods are usually derived from a generating function [8–10]. We derived the time-centered leapfrog from a variational principle (Hamilton's principle) and the ease of obtaining time-reversible and symplectic methods by that route was stressed by Miller and Prendergast [1] and again by Miller [2]. An exact Liouville theorem was emphasized in those papers.

The result displayed here with the predictor-corrector is unusual in the sense that a given method performs differently with different problems. The predictor-corrector performs well with the harmonic oscillator, but it yields unphysical results with the physical pendulum. The two problems seem quite similar from a numerical point of view. This feature of numerical methods, a sensitivity to the problem with which the method is to be used, need not show up by conventional means of analyzing the stability of numerical integration methods. Something more than mere smoothness and differentiability are required. It does, however, show up in the check for a symplectic method, which takes the actual forces into account. This is but one example of bizarre effects that can arise in numerical treatment of simple dynamical systems. Friedman and Auerbach [11, 12] show some other effects.

The predictor-corrector provides an example that shows how methods that look reliable can lead to unphysical predictions. Extreme care is needed in long or fussy integrations. And an integration can be fussy even though it appears quite straightforward. Who would have thought that the physical pendulum would harbor such surprises?

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