DIRECT MEASUREMENT OF LYAPUNOV EXPONENTS

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Benettin, Calgani and Strelcyn studied the dynamical separation of neighboring phase-space trajectories, determining the corresponding Lyapunov exponents by discrete rescaling of the intertrajectory separation. We incorporate rescaling directly into the equations of motion, preventing Lyapunov instability by using an effective constraint force.

The separation of phase-space trajectories with time is intimately connected to thermodynamic irreversibility and the loss of information [1]. In low density gases, spatial correlations can be entirely lost between collisions. Boltzmann's equation, and the H-theorem, correctly describe this regime. Although the basic mechanism for irreversibility was understood well by Boltzmann, quantitative calculations remained tedious until fast computers became available after the second world war. This new tool reawakened interest in the 19th century ideas of Boltzmann, Lyapunov, and Poincaré.

Thus, in 1967, Benettin, Galgani and Strelcyn developed a numerical means for measuring the time-evolution of the separation of neighboring phase-space trajectories [2]. Their method requires sufficiently smooth equations of motion, the solutions of which are trajectories, $r(t)$, in phase space.

Numerical solutions are necessarily approximate. This is because the differential equations of motion are replaced by approximate difference equations. The compounded errors in the difference-equation solutions soon destroy the mathematical reversibility of the original differential equations. The exponentially fast error growth is just a symptom of the underlying "Lyapunov instability". Benettin's investigations indicate that, despite this instability, the growth rate can be characterized reliably. Fundamentally, this is because fluctuations in the time-averaged growth rate are insensitive to initial conditions.

Lyapunov instability can be characterized quantitatively by following a pair of approximate trajectories whose separation satisfies two criteria: (i) it substantially exceeds the numerical resolution, while (ii) it is small relative to the radius of curvature of the trajectory. An unperturbed "reference trajectory", trajectory 1, is allowed to develop in time according to the given equations of motion. A second trajectory, offset from the reference trajectory and called "trajectory 2" is then kept "close" to trajectory 1 by a periodic scaling of its "coordinates". If we denote the coordinates of the reference and offset trajectories by r_1 and r_2, where each r represents the complete set of spatial coordinates and momenta $\{q,p\}$ describing the state of the system, the Benettin–Calgani–Strelcyn recipe for rescaling r_2, to give r_2', after scaling is as follows:

$$r_2' = r_2 - \alpha(r_2 - r_1)\,. \tag{1}$$

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The scale variable α is chosen to reduce $|r_2 - r_1|$ to its original offset length: If the scaling procedure is carried out at intervals dt, then Benettin, Galgani and Strelcyn show that the maximum Lyapunov exponent is, for sufficiently small offset and dt, just the quotient α/dt. Thus, the rate at which trajectories separate without scaling can be inferred directly from the scaling process.

During the past ten years a new kind of atomistic mechanical simulation, "nonequilibrium molecular dynamics", has developed as a useful computational and theoretical tool for simulating systems far from equilibrium [3]. An early difficulty in nonequilibrium simulations was maintaining a steady state. The natural conversion of work to heat in irreversible processes led to relatively rapid changes of state. This irreversible heating could be prevented [4] by rescaling the particle momenta, relative to the desired mean, p_0, from time to time

$$p' = p - \alpha(p - p_0) . \tag{2}$$

Eventually it became clear [5,6] that this rescaling could be carried out in a continuous way. To do this, a continuously varying constraint force, F_c, was added to the equations of motion:

$$\dot{p} = F(q) + F_c , \quad F_c = -\alpha(p - p_0) . \tag{3}$$

This same form (3), linear in the momenta, has since been justified on fundamental mechanical and statistical grounds [5–10] and has substantially simplified theoretical analyses of systems far from equilibrium [11].

The simplest "interesting system" to which the new equations can be applied is the one-dimensional harmonic oscillator. These equations [10,12] describe an oscillator at constant temperature rather than constant energy. They have the form:

$$\dot{q} = p , \quad \dot{p} = -q - \epsilon\xi p , \quad \dot{\xi} = \epsilon(p^2 - 1) , \tag{4}$$

where ϵ is a measure of the deviation of the trajectory from the newtonian limit, $\epsilon = 0$. A thorough investigation of this system is in progress [12]. The chaotic nature of some of the oscillator orbits has been characterized using Benettin's recipe as well as a simple continous scaling which maintains the inter-trajectory separation fixed. Because the latter continuous rescaling is conceptually simpler, it seems to us worthwhile to apply it to other like problems.

It is possible to include the phase-space scaling in the first-order ordinary differential equations of motion, just as was done for the momenta in (2) and (3) above. The result is

$$\dot{r}_2(\text{scaled}) = \dot{r}_2(r_2) - \alpha(r_2 - r_1) ,$$

$$\alpha = (r_2 - r_1)[\dot{r}_2(r_2) - \dot{r}_1(r_1)]/(r_2 - r_1)^2 . \tag{5}$$

This phase-space scaling and that of ref. [2] become identical as the time interval between rescalings approaches zero: Using this trajectory constraint is advantageous because it avoids the limiting process of a finite-difference approach and simplifies understanding. Provided that the equation of motion describing the reference trajectory is time-reversible, eqs. (5), for trajectory 2, are likewise reversible. It is convenient, in applications, to augment the equations of motion for the two trajectories with an additional equation integrating α with respect to time. At the conclusion of the calculation, the "Lyapunov exponent" $1/\tau$ is obtained by dividing this time integral of α by the total ellapsed time.

We have tested this continuous scaling by applying it to the Hénon–Heiles test case studied in ref. [2]. The results we found appear in table 1 and are fully consistent with graphical data presented in fig. 7 of ref. [2].

Benettin later pointed out (see the final footnote in ref. [2]) the possibility of measuring *all* the Lyapunov coefficients, not just the biggest, by following the distortion of a set of orthonormal basis vectors embedded in the flow. It is clear that this extension of the present suggestion could be implemented too.

Table 1
Lyapunov exponents $1/\tau$ for the Hénon–Heiles problem of ref. [2]. Initial conditions: $Q = 0.25$, $q = 0$, $P = 0.30$, and $p > 0$ as calculated from the hamiltonian $E = H = (Q^2 + q^2 + P^2 + p^2)/2 - Q^3/3 + Qq^2$. Each calculation was followed for one million time steps using the fourth-order Runge–Kutta method and a time step of 1/64. The separation between the two trajectories was held fixed at 0.0003.

E	$1/\tau$
0.105	0.030
0.115	0.035
0.125	0.049
0.135	0.066
0.145	0.085

Following Benettin's work Shimada and Nagashima developed numerical methods for determining the Lyapunov exponents in the limit that the trajectory offset vanishes [13]. The present finite offset may prove to be useful in stabilizing the long-time divergence problems associated with numerical linear-response theory [14]. This possibility emerged in discussions with D. Frenkel and G. Ciccotti at a 1985 CECAM meeting on "Nonequilibrium molecular dynamics" organized by Ciccotti and me.

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